A MICROMECHANICAL STUDY OF THE DAMAGE
MECHANICS OF ACRYLIC PARTICULATE COMPOSITES
UNDER THERMOMECHANICAL LOADING

By

Shihua Nie

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TABLE OF CONTENTS

ACKNOWLEDGEMENTS.......................................................................................................... ii

LIST OF FIGURES ........................................................................................................... ix

LIST OF TABLES ......................................................................................................... xxvi

ABSTRACT ...................................................................................................................... xxvii

CHAPTER 1  Introduction.................................................................................................. 1

  1.1 General ...................................................................................................................... 1
  1.2 Statement of the Problem .......................................................................................... 2
  1.3 Scope of Research ..................................................................................................... 5

CHAPTER 2  Literature Review ........................................................................................ 9

  2.1 Particulate Composites ............................................................................................ 9
    2.1.1 Mechanical Properties of Particulate Composites ......................................... 10
    2.1.2 Failure Mechanisms of Particulate Composites .............................................. 18
    2.1.3 Residual Stresses in Particulate Composites ............................................... 24
  2.2 Damage Mechanics ................................................................................................. 29
    2.2.1 Types of Damage ............................................................................................. 30
    2.2.2 Measurements of Damage ............................................................................ 32
    2.2.3 Cumulative Fatigue Damage ........................................................................... 36
      2.2.3.1 Fatigue Damage Related Parameters ........................................................ 37
      2.2.3.2 Linear Elastic Fracture Mechanics (LEFM) Models ................................ 39
      2.2.3.3 Continuum Damage Mechanics Models ................................................... 40
      2.2.3.4 Energy Based Approach ........................................................................... 41
2.3 Micromechanics of Particulate Composites

CHAPTER 3 Damage Evolution Function

3.1 Introduction

3.2 Conservation Laws

3.2.1 Conservation of Mass

3.2.2 Momentum Principle

3.2.3 Conservation of Energy

3.3 Entropy Law and Entropy Balance

3.4 Fully Coupled Thermal-Mechanical Equations

3.5 Damage Evolution Function

3.6 Damage Coupled Viscoplasticity

3.6.1 Effective Stress and Strain Equivalence Principle

3.6.2 Damage Coupled Isotropic Viscoelasticity

3.6.2.1 Damage Coupled Constitutive Equations

3.6.2.2 Damage Coupled Yield Surface

3.7 Examples

3.7.1 Damage Coupled Plasticity with Isotropic Hardening

3.7.2 Damage Coupled Plasticity with Linear Kinematic Hardening

CHAPTER 4 Damage Coupled Constitutive Model of Particulate Composites

4.1 Introduction

4.2 Ensemble-Volume Averaged Micromechanical Field Equations

4.3 Noninteracting Solution for Two-Phase Composites

4.3.1 Average Stress Norm in Matrix
4.3.2 Average Stress in Particles................................................................. 118
4.4 Pairwise Interacting Solution for Two-Phase Composites .................. 120
  4.4.1 Approximate Solution of Two-Phase Interaction ......................... 120
  4.4.2 Average Stress Norm in Matrix ...................................................... 124
  4.4.3 Average Stress in Particles............................................................... 127
4.5 Noninteracting Solution for Three-Phase Composites ....................... 129
  4.5.1 Effective Elastic Modulus of Multiphase Composites ..................... 130
  4.5.2 Average Stress Norm in Matrix ...................................................... 131
  4.5.3 Average Stress in Particles............................................................... 136
4.6 Effective Thermomechanical Properties of Composite Sphere Assemblage ...... 138
  4.6.1 Effective Bulk Modulus................................................................. 139
  4.6.2 Effective Coefficient of Thermal Expansion (ECTE) ...................... 140
  4.6.3 Effective Shear Modulus................................................................. 140
  4.6.4 Effective Young's Modulus and Poisson's Ratio ......................... 142
  4.6.5 Numerical Examples................................................................. 142
4.7 Micromechanical Model of Particulate Composites ........................... 149
  4.7.1 Modeling Procedures for Particulate Composites ......................... 150
  4.7.2 Elastic Properties of Particulate Composites ................................. 154
  4.7.3 Damage Coupled Viscoplasticity ................................................. 159
    4.7.3.1 Loading Function .............................................................. 159
    4.7.3.2 Damage Evolution ............................................................. 162
    4.7.3.3 Computational Integration Algorithm .................................. 163
    4.7.3.4 Consistent Elastoviscoplastic Tangent Modulus .................. 169
CHAPTER 5  Experiments ............................................................................................. 173

5.1 Introduction........................................................................................................... 173

5.2 Experimental Procedures ...................................................................................... 175

5.2.1 Nano Indentation Tests .................................................................................. 175

5.2.2 Mechanical Tests ........................................................................................... 176

5.3 Results and Discussions........................................................................................ 177

5.3.1 Failure Mechanism of Particulate Composites .............................................. 177

5.3.2 Nano Indentation Tests .................................................................................. 187

5.3.3 Monotonic Uniaxial Tests.............................................................................. 189

5.3.3.1 Influence of Strain Rates......................................................................... 190

5.3.3.2 Influence of Temperatures ...................................................................... 196

5.3.3.3 Comparison between Flexural and Tensile Tests ................................... 198

5.3.3.4 Influence of Interfacial Bonding Strength .............................................. 200

5.3.4 Loading and Unloading Tests ........................................................................ 203

5.3.5 Strain-Controlled Fatigue Tests ................................................................. 208

5.3.5.1 Stress-Strain Hysteresis Loops ............................................................... 209

5.3.5.2 Endurance Curve..................................................................................... 218

5.3.5.3 Damage Measurement ............................................................................ 220

5.3.5.3.1 Elastic Modulus Degradation........................................................... 220

5.3.5.3.2 Load Drop........................................................................................ 225

5.3.5.3.3 Plastic Strain Range ......................................................................... 230

5.3.5.3.4 Hysteresis Dissipation...................................................................... 234

5.3.6 Thermal Cycling Tests ................................................................................... 238
6.3.2 Finite Element Simulation Results ................................................................. 301
6.3.3 Parametric Studies ......................................................................................... 305
6.4 Cyclic Stress-Strain Response .............................................................................. 316
  6.4.1 Kinematic Hardening Parameters ................................................................. 317
  6.4.2 Finite Element Simulation Results ................................................................. 322
  6.4.3 Parametric Studies ......................................................................................... 328
6.5 Thermal Cycling of a Composite Plate with a Cutout ........................................ 334
  6.5.1 Model Parameters .......................................................................................... 335
  6.5.2 Finite Element Simulation Results ................................................................. 337
  6.5.3 Redesign of a Composite Plate with a Cutout ............................................... 346
CHAPTER 7  Conclusions and Recommendations ....................................................... 352
  7.1 Conclusions ........................................................................................................... 352
  7.2 Recommendations ................................................................................................. 356
  7.3 Contributions ......................................................................................................... 358
APPENDIX .................................................................................................................. 359
REFERENCES ............................................................................................................. 361
LIST OF FIGURES

Figure 1.1     Cracks near the drain hole of a kitchen sink made with an acrylic particulate composite ................................................................. 4

Figure 2.1     Schematic of particulate composites subjected to uniaxial tension: (A) undamaged; (B) damaged by debonding at the apex; (C) damaged by cavity formation (Ravichandran and Liu, 1995) ........................................... 21

Figure 2.2     Uniaxial stress-strain response and dilation as a function of strain (Ravichandran and Liu, 1995) ................................................................. 22

Figure 2.3     Schematic representation of (A) microhomogeneous; (B) craze-like deformation (Oshmyan and Muravin, 1997) ........................................... 23

Figure 2.4     Stress fringes when cooling ATH/PMMA composite ........................................ 28

Figure 2.5     Spring layer model (Hashin, 1991) ............................................................. 46

Figure 3.1     Schematic illustration of definition of damage ........................................... 80

Figure 3.2     Yield locus in the principal stress space (Lemaitre, et al., 1990) .................. 84

Figure 4.1     Effective Young’s modulus as a function of particle volume fraction ...... 104

Figure 4.2     Three-phase composite system ............................................................. 138

Figure 4.3     Schematic illustration of composite spherical assemblage (CSA) ............. 139

Figure 4.4     Variation of effective CTE with the interface parameter $q$ ................. 144

Figure 4.5     Variation of effective shear modulus with the interface parameter $q$ ...... 145

Figure 4.6     Variation of effective Young’s modulus with the interface parameter $q$ ................................................................................................. 146

Figure 4.7     Variation of effective bulk modulus with the interface parameter $q$ ...... 147
Figure 4.8  Variation of effective Poisson’s ratio with the interface parameter $q$ ...... 148
Figure 4.9  Modeling procedures – step 1: simplification ........................................... 151
Figure 4.10 Modeling procedures – step 2: equivalence ............................................ 152
Figure 4.11 Modeling procedures – step 3: thermomechanical properties ..................... 153
Figure 4.12 Modeling procedures – step 4: micromechanics ...................................... 154
Figure 4.13 Effective Young’s modulus vs. interface parameter at volume fraction
of 48% (The thickness of interphase is 1/10 of the diameter of particles).......................... 157
Figure 4.14 Effective Young’s modulus vs. interface parameter at volume fraction
of 48% (The thickness of interphase is 1/100 of the diameter of particles).......................... 158
Figure 4.15 Effective Young’s modulus vs. interface parameter at volume fraction
of 48% (The thickness of interphase is 1/1000 of the diameter of particles)......................... 159
Figure 4.16 A geometric interpretation of the closest point projection algorithm in stress space (Simo and Hughes, 1998) .................................................... 169
Figure 5.1 Specimen geometries for Nano indentation tests (mm) ......................... 175
Figure 5.2 Specimen geometries for mechanical tests (mm) .................................. 177
Figure 5.3 Polished surface of composite A (gray regions are particles) ............ 178
Figure 5.4 Particles in the PMMA/ATH system ..................................................... 179
Figure 5.5 Tensile fracture surfaces of composite A at room temperature .......... 181
Figure 5.6 Tensile fracture surfaces of composite A at 50 °C .............................. 181
Figure 5.7 Tensile fracture surfaces of composite A at 75 °C .............................. 182
Figure 5.8  Tensile fracture surfaces of composite A at 90 °C ................................. 182
Figure 5.9  Tensile fracture surfaces of composite B at room temperature .......... 183
Figure 5.10 Tensile fracture surfaces of composite B at 50 °C ............................... 183
Figure 5.11 Tensile fracture surfaces of composite B at 75 °C ............................... 184
Figure 5.12 Tensile fracture surfaces of composite C at room temperature .......... 184
Figure 5.13 Tensile fracture surfaces of composite C at 50 °C ............................... 185
Figure 5.14 Tensile fracture surfaces of composite C at 75 °C ............................... 185
Figure 5.15 Schematic of microdamage evolution in composite A and composite B.. 187
Figure 5.16 Schematic of microdamage evolution in composite C (Moshev and Evlampieva, 1997) .................................................................................... 187
Figure 5.17 Comparison of Young’s modulus of composite A as measured from uniaxial tensile tests with that from Nano Indenter® tests ......................... 189
Figure 5.18 Uniaxial tensile stress-strain curves of composite A at room temperature for different strain rates until failure .............................................. 191
Figure 5.19 Uniaxial tensile stress-strain curves of composite C at room temperature for different strain rates until failure .............................................. 192
Figure 5.20 Compressive stress-strain curves of composite A at room temperature for different strain rates until strain of 0.008 .............................................. 194
Figure 5.21 Compressive stress-strain curves of composite C at room temperature for different strain rates until strain of 0.01 ............................................... 194
Figure 5.22 Compressive stress-strain curves of composite A at displacement control rate of 5×10⁻³ mm/s and room temperature until buckling ............... 195
Figure 5.23  Stress-strain curves of composite A for one cycle with maximum strain 0.76% at different strain rates and room temperature ..................... 195

Figure 5.24  Uniaxial stress-strain curves of composite A at different temperatures (Celsius scale) .................................................................................................. 197

Figure 5.25  Uniaxial stress-strain curves of composite B at different temperatures (Celsius scale) .................................................................................................. 197

Figure 5.26  Uniaxial stress-strain curves of composite C at different temperatures (Celsius scale) .................................................................................................. 198

Figure 5.27  Comparison of stress-strain curve of composite A between uniaxial test and 3-point bending test at room temperature .............................................. 199

Figure 5.28  Uniaxial stress-strain curves of composite A, composite B and composite C at strain rate of $1 \times 10^{-4}/s$ and room temperature............................. 202

Figure 5.29  Uniaxial stress-strain curves of composite A, composite B and composite C at strain rate of $1 \times 10^{-4}/s$ and 50 °C ......................................................... 202

Figure 5.30  Uniaxial stress-strain curves of composite A, composite B and composite C at strain rate of $1 \times 10^{-4}/s$ and 75 °C ......................................................... 203

Figure 5.31  Uniaxial loading and unloading test for composite A at strain rate of $1 \times 10^{-4}/s$ and room temperature......................................................... 204

Figure 5.32  Uniaxial loading and unloading tests for composite A at strain rate of $1 \times 10^{-4}/s$ and temperature 50 °C ......................................................... 205

Figure 5.33  Uniaxial loading and unloading tests for composite A at strain rate of $1 \times 10^{-4}/s$ and temperature 75 °C ......................................................... 206
Figure 5.34  Uniaxial loading and unloading tests for composite A at strain rate of 
1×10^{-4} /s and temperature 75 °C ................................................................. 207

Figure 5.35  Strength degradation of composite A due to loading and unloading at 
the strain rate of 1×10^{-4} /s and 50 °C ............................................................. 208

Figure 5.36  Hysteresis loops for composite A at room temperature with strain 
amplitude of 0.425% (fails at cycle 1270). Plot for cycle 1, 10, 100, 
1270 .................................................................................................................. 210

Figure 5.37  Hysteresis loops for composite A at room temperature with strain 
amplitude of 0.6% (fails at cycle 104). Plot for cycle 1, 5, 10, 20, 30, 
40, 50, 60, 70, 80, 90, 104 .............................................................................. 211

Figure 5.38  Hysteresis loops for composite A at room temperature with strain 
amplitude of 0.68% (fails at cycle 24) ............................................................. 211

Figure 5.39  Hysteresis loops for composite A at 50 °C with strain amplitude of 
0.6% (fails at cycle 210). Plot for cycle 1, 5, 10, 20, 50, 100, 150, 180, 
200, and 210 .................................................................................................. 212

Figure 5.40  Hysteresis loops for composite A at 75 °C with strain amplitude of 
0.6% (fails at cycle 495). Plot for cycle 1, 5, 10, 20, 50, 100, 200, 300, 
400, 450, 480, and 495 ............................................................................... 212

Figure 5.41  Hysteresis loops for composite B at room temperature with strain 
amplitude of 0.6% (fails at cycle 23). Plot for cycle 1, 5, 10, 15, 20, 
23 .................................................................................................................... 213

Figure 5.42  Hysteresis loops for composite B at 50 °C with strain amplitude of 
0.6% (fails at cycle 38). Plot for cycle 1, 5, 10, 15, 25, 30, 35, 38 .......... 213
Figure 5.43  Hysteresis loops for composite C at room temperature with strain 
amplitude of 0.6% (fails at cycle 5292). Plot for cycle 1, 5, 10, 100, 
500, 1000, 2000, 3000, 4000, 4500, 5000, 5100, 5200, 5250, and 5292 .. 214

Figure 5.44  Hysteresis loops for composite C at 50 °C with strain amplitude of 
0.6% (fails at cycle 8156). Plot for cycle 1, 5, 10, 100, 2000, 
3000, 4000, 5000, 6000, 7000, 7500, 8000, 8100, and 8156 ............. 215

Figure 5.45  $S - N$ diagram for composite A and composite B at room temperature 
(strain rate for the fatigue tests is 0.01/s) .......................................... 219

Figure 5.46  Schematic illustration of measurement of unloading modulus .......... 221

Figure 5.47  Damage parameter $D$ as a function of number of cycles up to failure 
at different temperatures (in Celsius) with strain amplitude of 0.6% for 
composite A.............................................................................................. 222

Figure 5.48  Damage parameter $D$ as a function of number of cycles up to failure 
at room temperature (in Celsius) with different amplitudes for 
composite A.............................................................................................. 223

Figure 5.49  Damage parameter $D$ as a function of number of cycles up to failure 
at different temperatures (in Celsius) with strain amplitude of 0.6% for 
composite B.............................................................................................. 223

Figure 5.50  Damage parameter $D$ as a function of number of cycles up to failure 
at different temperatures (in Celsius) with strain amplitude of 0.6% for 
composite C.............................................................................................. 224
Figure 5.51  Damage parameter $D$ as a function of number of cycles up to failure at room temperature with strain amplitude of 0.6% for composite A and B ................................................................. 224

Figure 5.52  Comparison between definition 1 and definition 2 of load-drop parameter for composite A at room temperature and strain amplitude of 0.006................................................................. 226

Figure 5.53  Load-drop parameter (definition 1) as a function of number of cycles up to failure at different temperatures with strain amplitude of 0.6% for composite A ................................................................. 227

Figure 5.54  Load-drop parameter (definition 1) as a function of number of cycles up to failure at room temperature with strain amplitude of 0.6% for composite A ................................................................. 228

Figure 5.55  Load-drop parameter (definition) as a function of number of cycles up to failure at different temperatures with strain amplitude of 0.6% for composite B ................................................................. 228

Figure 5.56  Load-drop parameter (definition 1) as a function of number of cycles up to failure at different temperatures with strain amplitude of 0.6% for composite C ................................................................. 229

Figure 5.57  Load-drop parameter (definition 2) as a function of number of cycles up to failure at different temperatures with strain amplitude of 0.6% for composite C ................................................................. 229

Figure 5.58  Schematic definition of plastic strain range ............................................. 230
Figure 5.59  Plastic strain range as a function of number of cycles up to failure at
different temperatures (in Celsius) with strain amplitude of 0.6% for
composite A........................................................................................................ 231

Figure 5.60  Load-drop parameter as a function of number of cycles up to failure at
room temperature with different amplitudes for composite A.................. 232

Figure 5.61  Plastic strain range as a function of number of cycles up to failure at
different temperatures (in Celsius) with strain amplitude of 0.6% for
composite B........................................................................................................ 232

Figure 5.62  Plastic strain range as a function of number of cycles up to failure at
different temperatures with strain amplitude of 0.6% for composite C .... 233

Figure 5.63  Hysteresis dissipation as a function of number of cycles up to failure
at different temperatures (in Celsius) with strain amplitude of 0.6% for
composite A........................................................................................................ 234

Figure 5.64  Hysteresis dissipation as a function of number of cycles up to failure
at room temperature with different amplitudes for composite A .............. 235

Figure 5.65  Hysteresis dissipation as a function of number of cycles up to failure
at different temperatures (in Celsius) with strain amplitude of 0.6% for
composite B........................................................................................................ 235

Figure 5.66  Hysteresis dissipation as a function of number of cycles up to failure
at different temperatures (in Celsius) with strain amplitude of 0.6% for
composite C........................................................................................................ 236
Figure 5.67  Cumulative hysteresis dissipation as a function of number of cycles up to failure at various temperatures (in Celsius) with strain amplitude of 0.6% for composite A................................................................. 237

Figure 5.68  Temperature profile for the thermal fatigue test........................... 238

Figure 5.69  First 3-cycle stress-strain responses for composite A under the thermal fatigue test ................................................................. 239

Figure 5.70  Total strain as a function of time for composite A with various tensile loads at 22 °C as plotted on (A) logarithmic and (B) linear time scales ... 242

Figure 5.71  Total strain as a function of time for composite A with various tensile loads at 50 °C as plotted on (A) logarithmic and (B) linear time scales ... 243

Figure 5.72  Total strain as a function of time for composite A with various tensile loads at 75 °C as plotted on (A) logarithmic and (B) linear time scales ... 244

Figure 5.73  Creep strain as a function of time for composite A with various tensile loads at 22 °C as plotted on (A) logarithmic and (B) linear time scales ... 245

Figure 5.74  Creep strain as a function of time for composite A with various tensile loads at 50 °C as plotted on (A) logarithmic and (B) linear time scales ... 246

Figure 5.75  Creep strain as a function of time for composite A with various tensile loads at 75 °C as plotted on (A) logarithmic and (B) linear time scales ... 247

Figure 5.76  Creep strain rate as a function of time for composite A with various tensile loads at 22 °C as plotted on (A) logarithmic and (B) linear time scales ................................................................. 248
Figure 5.77 Creep strain rate as a function of time for composite A with various
tensile loads at 75 °C as plotted on (A) logarithmic and (B) linear time
scales ............................................................................................................... 249

Figure 5.78 Effects of stress on the stationary creep strain rate of composite A at
75 °C as plotted on (A) logarithmic and (B) linear stationary creep
strain rate scales ........................................................................................ 251

Figure 5.79 Effects of temperature on the creep strain of composite A at stress of
25 MPa as plotted on (A) logarithmic and (B) linear time scales ............. 252

Figure 5.80 Creep strain in tension and compression for composite A at 22 °C as
plotted on (A) logarithmic and (B) linear time scales ......................... 254

Figure 5.81 Creep strain rate in tension and compression for composite A at 22 °C
as plotted on (A) logarithmic and (B) linear creep strain rate scales ....... 255

Figure 5.82 Creep strain in tension and compression for composite A at 75 °C as
plotted on (A) logarithmic and (B) linear time scales ......................... 257

Figure 5.83 Creep strain rate in tension and compression for composite A at 75 °C
as plotted on (A) logarithmic and (B) linear creep strain rate scales ....... 258

Figure 5.84 Examples illustrating the use of a second (compensating) strain gage
in an adjacent Wheatstone bridge arm to cancel the effect of thermal
output ............................................................................................................... 268

Figure 5.85 Dimension of the composite plate with a cutout (mm) .................... 272

Figure 5.86 Distribution of the temperature control points ............................. 272

Figure 5.87 Distribution of the strain gage points ............................................. 273

Figure 5.88 Temperature profile at the temperature control points............... 274
Figure 5.89   USB temperature data acquisition system................................................. 275
Figure 5.90   Thermal plate used to heat strain gage/composite assembly............... 275
Figure 5.91   Thermal output measurement system....................................................... 275
Figure 5.92   Thermal strain as a function of temperature for strain gage EA-13-
               125AC-350/composite assembly............................................................... 276
Figure 5.93   Thermal strain as a function of temperature for strain gage EA-13-
               031DE-350/composite assembly............................................................... 277
Figure 5.94   Thermal strain as a function of temperature for strain gage EA-13-
               125RD-350/composite assembly............................................................... 277
Figure 5.95   Strain gage locations.................................................................................. 278
Figure 5.96   Strain in strain gage a as a function of time for test #2 ......................... 279
Figure 5.97   Maximum strain in strain gage b as a function of time for test #2 .......... 280
Figure 5.98   Minimum strain in strain gage b as a function of time for test #2.......... 280
Figure 5.99   Maximum strain in strain gage b' as a function of time for test #2 ......... 281
Figure 5.100  Minimum strain in strain gage b' as a function of time for test #2 ......... 281
Figure 5.101  Maximum strain in strain gage b as a function of time for test #3 ........... 282
Figure 5.102  Minimum strain in strain gage b as a function of time for test #3 ........... 282
Figure 5.103  Maximum strain in strain gage c as a function of time for test #3 .......... 283
Figure 5.104  Minimum strain in strain gage c as a function of time for test #3 .......... 283
Figure 5.105  Strain in strain gage d as a function of time for test #3 ....................... 284
Figure 5.106  Strain in strain gage f as a function of time for test #3 ...................... 284
Figure 5.107  Strain in strain gage e as a function of time for test #2 ...................... 285
Figure 5.108  Strain in strain gage e' as a function of time for test #2..................... 285
Figure 5.109  Strain in strain gage e' and strain gage e* as a function of time for test #1 after cycle 21 ................................................................. 286

Figure 5.110  Cracks near the corner of cutout in the composite plate .......................... 287

Figure 5.111  Temperature distribution in plate around heating source when the maximum temperature of controlled points is 120 °C .......................... 287

Figure 6.1  Young's modulus of PMMA as a function of temperature (Cheng et al., 1990) ................................................................. 292

Figure 6.2  Poisson’s ratio of composite A as a function of temperature .................. 293

Figure 6.3  Coefficient of thermal expansion (CTE) of composite A as a function of temperature ................................................................. 294

Figure 6.4  Relaxation time of composite A as a function of temperature ................. 295

Figure 6.5  Elastic modulus of Composite A as a function of temperature .............. 296

Figure 6.6  Stress as a function of viscoplastic strain at various temperatures ........ 298

Figure 6.7  Initial yield stress of composite A as a function of temperature ............ 299

Figure 6.8  Parameter K of composite A as a function of temperature .................... 299

Figure 6.9  Parameter n of composite A as a function of temperature ................. 300

Figure 6.10  Critical damage parameter of composite A as a function of temperature .................................................................................. 301

Figure 6.11  Comparison of stress-strain relationship among damage coupled viscoplastic model, viscoplasticity model without and experiment data at 24°C ........................................................................................................ 302

Figure 6.12  Comparison of stress-strain relationship among damage coupled viscoplastic model, viscoplasticity model and experiment data at 75°C... 303
Figure 6.13 Comparison of damage parameter obtained from damage model with that measured in experiments in terms of elastic modulus degradation at 24°C ................................................................. 304

Figure 6.14 Comparison of damage parameter obtained from damage model with that measured in experiments in terms of elastic modulus degradation at 75°C ................................................................. 305

Figure 6.15 Effect of the CTE mismatch between the matrix and the particle on the stress-strain relation of composite A at 24°C ....................................................... 306

Figure 6.16 Effect of the CTE mismatch between the matrix and the particle on the stress-strain relation of composite A at 75°C ....................................................... 307

Figure 6.17 Effect of the stiffness of interphase around particle on the stress-strain relation of composite A at 24°C ................................................................. 308

Figure 6.18 Effect of the stiffness of interphase around particle on the stress-strain relation of composite A at 75°C ................................................................. 308

Figure 6.19 Effect of the thickness of interphase around particle on the stress-strain relation of composite A at 24°C ................................................................. 309

Figure 6.20 Effect of the thickness of interphase around particle on the stress-strain relation of composite A at 75°C ................................................................. 310

Figure 6.21 Effect of the yield strength of composite A on the stress-strain relation of composite A at 24°C ................................................................. 311

Figure 6.22 Effect of the yield strength of composite A on the stress-strain relation of composite A at 75°C ................................................................. 311
Figure 6.23  Effect of the particle volume fraction on the stress-strain relation of composite A at 24 °C ................................................................. 312

Figure 6.24  Effect of the particle volume fraction on the stress-strain relation of composite A at 75 °C ................................................................. 313

Figure 6.25  Effect of the elastic modulus of matrix on the stress-strain relation of composite A at 24 °C ................................................................. 314

Figure 6.26  Effect of the elastic modulus of matrix on the stress-strain relation of composite A at 75 °C ................................................................. 314

Figure 6.27  Effect of the elastic modulus of particle on the stress-strain relation of composite A at 24 °C ................................................................. 315

Figure 6.28  Effect of the elastic modulus of particle on the stress-strain relation of composite A at 75 °C ................................................................. 316

Figure 6.29  Displacement profile for strain-controlled fatigue tests .................................................. 317

Figure 6.30  The 1st cycle stress-strain curve in tension direction for the cyclic tests with the strain amplitude of 0.6% at room temperature .................. 318

Figure 6.31  Initial yield stress of composite A for the linear kinematic model as a function of temperature ................................................................. 319

Figure 6.32  The 5th cycle stress-strain curve in tension direction for the cyclic tests with the strain amplitude of 0.6% at room temperature ................. 320

Figure 6.33  Kinematic hardening modulus of composite A as a function of temperature ................................................................. 321

Figure 6.34  Uniaxial stress-strain hysteresis loop simulation vs. experimental data for cycle 5 at room temperature with strain amplitude of 0.6% ........ 323
Figure 6.35  Uniaxial stress-strain hysteresis loop simulation vs. experimental data for cycle 50 at room temperature with strain amplitude of 0.6%.............. 323

Figure 6.36  Uniaxial stress-strain hysteresis loop simulation vs. experimental data for cycle 104 at room temperature with strain amplitude of 0.6%............ 324

Figure 6.37  Uniaxial stress-strain hysteresis loop simulation vs. experimental data for cycle 5 at 75 °C with strain amplitude of 0.6% .......................... 324

Figure 6.38  Uniaxial stress-strain hysteresis loop simulation vs. experimental data for cycle 100 at 75 °C with strain amplitude of 0.6% ....................... 325

Figure 6.39  Uniaxial stress-strain hysteresis loop simulation vs. experimental data for cycle 495 at 75 °C with strain amplitude of 0.6% ......................... 325

Figure 6.40  Comparison of damage parameter obtained from damage coupled plastic model with that measured in experiments in terms of elastic modulus degradation at room temperature with strain amplitude of 0.6%................................................................. 326

Figure 6.41  Comparison of damage parameter obtained from damage coupled plastic model with that measured in experiments in terms of elastic modulus degradation at 75 °C with strain amplitude of 0.6%....................... 327

Figure 6.42  Effect of the CTE mismatch between the matrix and the particle on the damage of composite A at room temperature ................................. 328

Figure 6.43  Effect of the stiffness of interphase around particle on the damage of composite A at room temperature .............................................. 329

Figure 6.44  Effect of the thickness of interphase around particle on the damage of composite A at room temperature .............................................. 330
Figure 6.45 Effect of the yield strength of composite A on the damage of composite A at room temperature ............................................................. 331

Figure 6.46 Effect of the particle volume fraction on the damage of composite A at room temperature (Volume of Fratation (VoF)) .................................................. 332

Figure 6.47 Effect of the elastic modulus of matrix on the damage of composite A at room temperature .................................................................................. 333

Figure 6.48 Effect of the elastic modulus of particle on the damage of composite A at room temperature ................................................................. 334

Figure 6.49 schematic illustration of the half of composite plate with a cutout ........ 335

Figure 6.50 Initial yield stress of Composite A as a function of temperature .......... 336

Figure 6.51 Linear kinematic hardening modulus of composite A as a function of temperature ...................................................................................... 337

Figure 6.52 Comparison of simulations with experimental measurements for strain in the plane direction at the corners close to heat source for cycle 1 .... 338

Figure 6.53 Comparison of simulations with experimental measurements for strain in the plane direction at the corners close to heat source for cycle 5 .... 338

Figure 6.54 Comparison of simulations with experimental measurements for strain in the plane direction at the corners close to heat source for cycle 10 ...... 339

Figure 6.55 Comparison of simulations with experimental measurements for strain in the plane direction at the corners close to heat source for cycle 34 ...... 339

Figure 6.56 Damage distributions in the plate with cutout for cycle 1 ................. 341

Figure 6.57 Damage distributions in the plate with cutout for cycle 10 ............... 341

Figure 6.58 Damage distributions in the plate with cutout for cycle 34 ............... 342
Figure 6.59  von Mises stress distributions in the plate with cutout for cycle 1............ 343

Figure 6.60  von Mises stress distributions in the plate with cutout for cycle 10........... 343

Figure 6.61  von Mises stress distributions in the plate with cutout for cycle 34............ 344

Figure 6.62  Damage at the corners close to the heat source as a function of the number of cycles ....................................................................................... 345

Figure 6.63  von Mises stress at the corners close to the heat source as a function of the number of cycles ................................................................................. 345

Figure 6.64  Reinforcing steel plate on the inside surface of the corner ..................... 347

Figure 6.65  Reinforcing steel plate on the top and bottom surfaces of the corner ...... 347

Figure 6.66  von Mises stress distributions around the corner close to the heat source for design #1 ............................................................................................... 348

Figure 6.67  von Mises stress distributions around the corner close to the heat source for design #2 ......................................................................................... 349

Figure 6.68  von Mises stress distributions around the corner close to the heat source for design #3 ......................................................................................... 349

Figure 6.69  von Mises stress in the corner close to the heat source for the first cycle ............................................................................................................... 350

Figure 6.70  Damage evolution in the corner close to the heat source as a function of the number of cycles ............................................................................. 351

Figure 6.71  von Mises stress in the corner close to the heat source as a function of the number of cycles .................................................................................. 351
LIST OF TABLES

Table 5.1 Chemical and physical composition of the acrylic particulate composites .... 174

Table 5.2 Young’s modulus of composite A at room temperature from Nano Indenter® test ............................................................................................. 188

Table 5.3 Hardness of composite A at room temperature from Nano Indenter® test ..... 188

Table 6.1 Initial yield stress for linear kinematic model ................................................ 318

Table 6.2 Kinematic hardening modulus for linear kinematic model ............................ 320
The main aim of this dissertation was to characterize the damage mechanism and fatigue behavior of the acrylic particulate composite. This dissertation also investigated how the failure mechanism is influenced by changes in certain parameters including the volume fraction of particle, the interfacial bonding strength, the stiffness and thickness of the interphase, and the CTE mismatch between the particle and the matrix.

Monotonic uniaxial tensile and compressive testing under various temperatures and strain rates, isothermal low-cycle mechanical testing and thermal cycling of a plate with a cutout were performed. The influence of the interfacial bonding strength between the particle and the matrix on the failure mechanism of the ATH filled PMMA was investigated using in situ observations under uniaxial loading conditions. For composites with weak interfacial bonding, the debonding is the major damage mode. For composites with strong interfacial bonding, the breakage of the agglomerate of particles is the major damage mode. Experimental studies also demonstrated the significant influence of interfacial bonding strength on the fatigue life of the ATH filled PMMA. The damage was characterized in terms of the elastic modulus degradation, the load-drop parameter, the plastic strain range and the hysteresis dissipation.

Identifying the internal state variables that quantify material degradation under thermomechanical loading is an active research field. In this dissertation, the entropy production, which is a measure of the irreversibility of the thermodynamic system, is used as the metric for damage. The close correlation between the damage measured in terms of elastic modulus degradation and that obtained from the finite element simulation results validates the entropy based damage evolution function.
A micromechanical model for acrylic particulate composites with imperfect interfacial bonds was proposed. Acrylic particulate composites are treated as three-phase composites consisting of agglomerated particles, bulk matrix and an interfacial transition zone around the agglomerate. The influence of the interfacial bonding and the CTE mismatch between the matrix and the filler on the overall thermomechanical behavior of composites is studied analytically and experimentally. The comparison of analytical simulation with experimental data demonstrated the validity of the proposed micromechanical model for acrylic particulate composites with an imperfect interface.

A damage-coupled viscoplastic constitutive model was also developed to predict the thermomechanical behavior and fatigue life of the acrylic particulate composites. The damage coupled constitutive model simulates the interaction between damage and response of the composite material under thermomechanical loading. The material parameters involved in the constitutive model have been experimentally determined and been implemented into the commercial general-purpose finite element package ABAQUS through user-defined subroutines. The finite element simulation results agree well with the test data from monotonic uniaxial tensile tests and fatigue tests at various temperatures. It is shown that the proposed damage coupled viscoplastic constitutive model can be used to predict the fatigue life of an acrylic particulate composite under thermomechanical fatigue loading.
CHAPTER 1

Introduction

1.1 General

The rapid growth of the composites industry continues to create a need for materials that meet the demand for high performance at an economical cost. A particulate composite consists of a physical mixture of particles (fillers) and a binder material (matrix). Various combinations of particles and matrix can be used to produce the composite. The particle material can be metallic or nonmetallic and the same holds true for the binder material. Jones (1999) classifies particulate composites into four categories: nonmetallic particles in a nonmetallic binder, metallic particles in a nonmetallic binder, metallic particles in a metallic binder and nonmetallic particles in a metallic binder. In general, the addition of particles to matrix materials can produce a number of desirable effects. Nielsen (1967) summarized the practical reasons for the use of the fillers:

- To stiffen the matrix
- To regulate the coefficient of thermal expansion and thermal shrinkage of the material
- To improve heat resistance
- To reduce creep
- To increase the strength properties of the polymer or other matrix material
- To modify the permeability behavior to gases and liquids
- To improve electrical properties
- To modify rheological properties
- To lower the cost of the material
1.2 Statement of the Problem

Acrylic particulate composites are increasingly employed in a wide variety of domestic and industrial applications due to their low cost, nearly isotropic properties, ease of fabrication, favorable material properties and their enormous versatility and aesthetic qualities. But acrylic particulate composites are known to accumulate considerable scattered microscopic damage in their service life. The failure, when it occurs, comes on suddenly in materials that have accumulated some degree of damage and have altered their effective behavior. The compression and shear strength of the acrylic particulate composites is improved; however, fillers often decrease the tensile strength and ductility of the matrix. This low tensile stress and ductility and unfavorable combination of such properties as low thermal conductivity and relative high Young’s modulus of elasticity render acrylic particulate composite highly susceptible to fatigue under service loading conditions which promote the generation of high magnitude thermal stress.

Much of the focus in terms of applications for acrylic particulate composites has been in the solid surface industry, where they are gradually replacing traditional materials such as natural stone (marble), wood, particle board and laminated products in the manufacture of kitchen countertops, sinks, bathroom vanities and a variety of other applications. When kitchen countertops are provided with a cutout, generally rectangular in shape, in order to drop in an appliance such as a cooktop, there are potential problems with the corners of the cutout acting as stress risers. An appliance, such as a cooktop cycling through high and low temperatures, undergoes thermal cycling that causes the countertop to expand and contract. Depending on conditions, this thermal cycling can
eventually lead to the forming of cracks in the countertop corners, which might then propagate out into the countertop and cause failure.

Products such as fabricated kitchen sinks and bathroom vanities are also normally subjected to severe temperature variations due to alternating flows of hot and cold water. Again, these temperature variations may give rise to high thermal stress, which may sometimes lead to failure by causing cracks in the region near the drain hole. Recent studies of the kitchen sinks made from acrylic particulate composites indicate that cracks indeed occur close to the drain hole placed on the bottom of the sinks as shown in Figure 1.1. The cause of these fractures seems to be the thermal stress originating from severe temperature variations that occur when alternating flows of cold and hot water are applied.
Figure 1.1 Cracks near the drain hole of a kitchen sink made with an acrylic particulate composite
An understanding of the mechanisms by which acrylic particulate composite fails is needed both for material evaluation and as a basis for improving the design. Fatigue failure of acrylic particulate composites is an area of research that has received little prior attention, and related studies in the literature are generally scarce. In basic terms, fatigue could be referred to as a loss of strength, functional effectiveness or any other important property as a result of subjecting a material or structure to either static or dynamic loads over a period of time. Dynamic fatigue which is more important and more readily encountered, involves failure that occurs at relatively low stress levels in structures or materials. The investigations carried out here were necessary in order to provide a more in-depth understanding of failure behavior of acrylic particulate composites under service conditions.

1.3 Scope of Research

Based on the above considerations, the main work in this dissertation focused on the following:

1. Material testing of acrylic particulate composites

Material testing at different temperatures is one of the main foci of interest in this project. Monotonic uniaxial tensile tests and strain-controlled fatigue tests were conducted at different temperatures and various strain rates. The mechanical properties of composites, such as elastic modulus, yield stress, kinematic and isotropic hardening parameters were determined under different temperatures and different loading rates. The material degradation in fatigue was measured in terms of inelastic strain range, load-drop parameter, elastic modulus degradation, and dissipated strain energy. The creep
properties of an acrylic particulate composite were also determined experimentally through
traditional mechanical tests, and the observed characteristics of creep are presented.
Finally, thermomechanical testing were performed on the plate with a cutout in which a
heating tub was inserted. Mechanical strains and temperature distributions around the
cutout were measured *in-situ*.

2. Interfacial properties between the matrix and the filler

Information regarding the interaction between the matrix and the surface of the
reinforcement particle is important. Particle surface treatment is one way of changing the
interfacial adhesion between the matrix and the filler. In this dissertation, the composite
samples are prepared with the ductile lightly crosslinked poly-methyl methacrylate
(PMMA) and hard, brittle alumina trihydrate (ATH). The filler volume fraction, filler
size and filler shape are kept constant and the interfacial bond strength is the only
variable. For the test specimens, three kinds of interfacial adhesion between the matrix
and the filler were produced:

- There is chemical bonding agent between the particle and the matrix, resulting in a
  strong reinforcing effect (composite A).
- The matrix is bonded to the particle surface by self-reaction, thus resulting in a
  marked reinforcing effect. No adhesion promoting agent was used (composite B).
- There is a chemical debonding agent between the particle and the matrix, resulting in
  weak interfacial adhesion (composite C).

The great influence of interfacial bonding strength between the particle and the matrix on
the thermomechanical properties and failure modes of the particulate was studied
experimentally.
3. Failure mechanism of acrylic particulate composite

The mechanisms of failure in acrylic particulate composites were investigated using \textit{in situ} observations during tensile, compressive and cyclic loading at different temperatures and strain rates.

4. Damage evolution function

A damage evolution function was proposed to predict the damage status in the composites. For a solid system, the entropy production is a non-negative quantity based on irreversible thermodynamics and thus serves as a basis for the systematic description of the irreversible processes occurring in a solid. In this dissertation, a thermodynamic framework has been presented for damage mechanics of solid materials, where the internal entropy production is used as the sole measure of damage in the system. As a result, there is no need for physically meaningless empirical parameters to define a phenomenological damage potential function.

5. A micromechanical constitutive model for acrylic particulate composites

As information on the material and its properties was obtained along with an understanding of its response, tendencies and behavior under thermomechanical loadings, a micromechanical model for the effective elastic properties of acrylic particulate composites with imperfect interfacial bonds was proposed. In this dissertation, particle filled acrylic composites were treated as three-phase composites consisting of an agglomerate of particles, a bulk matrix and an interfacial transition zone around the agglomerate. The influence of the interfacial transition zone and the CTE mismatch between the matrix and the filler on the overall thermomechanical behavior of composites is studied analytically and experimentally. The comparison of analytical simulation with
experimental data was made to validate the proposed micromechanical model with imperfect interfaces.

6. Damage coupled viscoplasticity constitutive model

A damage coupled viscoplastic constitutive model based on micromechanics was also developed to predict mechanical fatigue life of acrylic particulate composites. The damage-coupled constitutive model reflects the interaction between the damage and the mechanical response of material under fatigue loading. The material parameters involved in the constitutive model were experimentally determined and have been implemented into the commercial finite element package ABAQUS through the user-defined subroutines.

7. Suggestions for improving the properties of particulate composites

Finally, recommendations were made for the development of acrylic particulate composite with improved thermal stress resistance as well as the directions to be taken in engineering design in order to reduce the susceptibility of acrylic particulate composite structures to thermal stress induced fatigue.
CHAPTER 2

Literature Review

2.1 Particulate Composites

When a ductile matrix is reinforced by elastic inclusions of high strength and high modulus, this leads to a number of desirable effects such as an increase in stiffness, a reduction in thermal expansion, an improvement in creep resistance and fracture toughness, and the improved compression and shear strength (compared with matrix). Although reinforcements could be continuous in the form of fibers or discontinuous in the form of particles or whiskers, the particle-reinforced ductile matrix composites are widely used as they can exhibit nearly isotropic properties (if randomly oriented) and are often easier to manufacture and process.

The microstructure of acrylic particulate composites consists of a distribution of particles in a continuous ductile matrix. In tension, the particles act as stress concentrators, while in compression the particles serve to transmit stress. The resulting material is brittle in tension, but in compression it is similar in behavior to a ductile matrix. Therefore, particulate composites usually exhibit markedly different inelastic behavior in tension and compression:

- Yield stress in tension is three to five times lower than the yield stress in compression.
- Permanent volume increases in tension, but negligible inelastic volume change in compression.
- Different hardening behavior in tension and compression.
Particulate composites are known to accumulate considerable scattered microscopic damage in their service life. Although the addition of rigid particles to polymers can produce desirable effects, fillers often decrease the tensile strength and ductility of this kind of material (compared with matrix). This low tensile strength and ductility and unfavorable combination of such properties as low thermal conductivity and relative high Young’s modulus of elasticity render acrylic particulate composites highly susceptible to fatigue under a service loading condition, which promotes the generation of high thermal stress. Common continuum mechanical equations expressing mechanical behavior of particulate composites are not able by themselves to predict the failure phenomenon, since a smooth evolution of the mechanical state changes to a sudden breakdown (Moshev and Evlampieva, 1997). For example, strength criteria are usually invoked to establish the state of material just before failure. In such an approach, strength criteria manifest themselves as some rather independent material variables. In this chapter, some of the relevant background, important experimental and essential theories that are required for an understanding of the work carried out in this dissertation are introduced and discussed.

2.1.1 Mechanical Properties of Particulate Composites

The most important characteristics for acrylic particulate composites are mechanical properties such as tensile strength, impact strength, and elongation at break. The strength of a composite is based on the nature of the matrix as well as on the interaction between the matrix and the particle. Therefore, it is important to understand the influence and role of the particles in the matrix for the development of composite
systems with improved properties. The important factors and considerations associated with polymer-filler systems are introduced and discussed in this chapter.

Many researchers, including Kwon (1995, 1997, 1998), Liu (1995, 1997, 1998), Lee (1997, 1998), Oshmyan and Muravin (1997), Miyano et al. (1999), Wong and Ait-Kadi (1997), have attempted to describe the behavior of acrylic particulate composites and the damage in these particulate composites macromechanically or micromechanically. These studies suggested that particles play an important role in the tensile strength of the composite.

In a two-phase composite made up of a continuous matrix and particulate fillers, the type, concentration, size, aspect ratio and distribution, elastic modulus, shape and orientation of the particles are important factors in determining the mechanical and physical properties. Among several other factors that can greatly affect the mechanical behavior of the filled systems, the strength of the adhesive bond between different phases, the type of dispersion and the amount of particle agglomeration are especially important. Unfortunately, these factors are often difficult to separate and to evaluate in a quantitative manner.

Modulus is one of the most basic mechanical properties of particulate composites. Modulus of a particulate composite depends on the volume fraction of the particle and other factors such as the size of fillers, and the interfacial bonding strength between the filler and the matrix. When the modulus of the filler is greater than that of the polymer, the modulus of the composite increases with increasing amount of fillers (assuming a perfect interfacial bond between the matrix and the particle). On the other hand, when the modulus of the filler is smaller than that of the polymer, the modulus of the composite
should decrease as increasing the amount of filler. The modulus may also have strong amplitude dependence so that above the critical amplitude of stress or strain, the modulus shows a rapid decrease. However, because of the volume occupied by the filler, the elongation of the polymer at failure is greater than the observed elongation of a specimen of the filled material (Nielsen, 1967). Generally, the particles embrittle the matrix; with the ductility being mainly dependent on the volume fraction of the particles, and relatively insensitive to particle shape and size. Studies by Nielsen (1967) also indicate that reinforcing action is nearly independent of the modulus of the filler as long as it is considerably greater than the modulus of the continuous phase.

The shape of the inclusion is also expected to play an important role in determining the strength of the filled system. With a irregularly shaped inclusion, the weakening is due to a high stress concentration coupled with a size effect, while for rounded cracks and inclusions, the stress concentration is much less severe than for inclusions with sharp corners. In the case of non-spherical particles, the degree of orientation with respect to applied stress is also important (Ferreira et al., 1997). In the theoretical derivation of filler reinforcement, the shape of the filler particle is assumed to be spherical. However, in reality, there are many filler particles that are not spherical; cylindrical and plate-like filler particles are commonly used. In general, as the filler particles depart from spherical to irregular shapes, the modulus reinforcement becomes larger.

Both the experimental data and the empirical model suggested by Papanicolaou et al. (1992) provide results that composites made with smaller filler particles have higher strength. The reason for this is not entirely clear, but the increasing interfacial area per
unit volume of filler for smaller filler particles must have a positive influence on the strength of the composite. In addition, as particle size decreases, the modulus and yield strength increase while the elongations at yield and at break decrease. Alter (1965) studied the relationship between the particle diameter of the filler and the modulus of acrylic particulate composites. The relative modulus was shown to correspond linearly to the reciprocal value of the particle diameter. Experimental evidence also suggests that the strength of polymer composites depend on the size as well as the volume fraction of the filler particles (London et al., 1977). The epoxy/glass composites’ strengths found by experiments for four different particle diameters (216 $\mu m$, 147 $\mu m$, 77 $\mu m$ and 21 $\mu m$) were compared with the corresponding values predicted by their model. This comparison shows that for the range of particle diameters studied, the composite strength diminishes at higher volume fractions.

The effect of irregularly shaped glass particle size and size distribution on the flexural mechanical properties of highly-filled composites with a rubbery thermoplastic matrix was studied by Kauly et al. (1996). Below is a summary of the conclusions that could be obtained from their experimental investigation:

- The median size of the particles has a pronounced effect on the composites' mechanical behavior. The flexural modulus and strength both increase, while the deflection at failure in flexure decreases with a decreasing median size. However, the size distribution width does not seem to affect the mechanical properties.

- The addition of a second particle population of different median size increases the flexural modulus and strength, and the brittleness. The increase is larger when the median size of the additional population is larger than that of the original powder.
The high glass particle content in the highly filled composites create, as a result of many contact points and mechanical interlocking, a kind of "glass network." The nature of this glass network is the dominant factor in determining the mechanical properties of the composite material. Particle size and shape, which define the specific surface area of the powder and, therefore, the number of contact points between the particles and degree of mechanical interlocking, have a dominating effect on the mechanical properties.

The flexural modulus, strength and ductility may be significantly enhanced by changing the surface properties of the glass particles. Increasing the polymer/glass particle bonding strength changes the mode of failure.

Another important factor that influences the mechanical properties of a particulate composite is the interfacial adhesion between the matrix and the filler. This interfacial property determines the interaction between the filler and the matrix. The mechanical behavior of polymer composites depends strongly on the adhesion between the polymer matrix and the filler. The layer of polymer that is in contact with the filler may have mechanical properties different from those of the rest of the matrix because of the interaction with the filler surface via electrostatic forces or chemical bonds, mechanical immobilization of the chains or because of the presence of internal stresses, voids, or microcracks in the interlayer. The properties of the interface may play an important role in determining the mechanical behavior of the composite. It was shown that an increase in adhesive strength leads to an increase in the ultimate strength at failure. In contrast, weakening the interface between the matrix and the filler results in a reduction in strength at failure. The nature of the adhesive bond at the interface between the two components of a composite material also has a profound effect on the elastic modulus of the system.
The poor particle-matrix bond will act as an inherent flaw with the production of a cavity equal to its size (Ferreira et al., 1997). However, the non-bonded particles may not act entirely as holes, since they also restrain the matrix from collapsing in compression. Therefore, the modulus of the filled system should increase with increasing filler content.

Kauly et al. (1996) also investigated the effect of particle/polymer interaction on the mechanical properties of polymer particulate composites, by treating the glass powder with two kinds of silane coupling agents. They found that the silane A-174 treatment had no effect on the mechanical properties and on the density of the composites, while the Ucarsil treatment had dramatic effects. Ucarsil had the effect of increasing the flexural strength by a factor of 1.7, the flexural modulus by a factor of 9, and doubling the deflection of the composites at failure.

In many practical applications, the individual fillers are not separated from one another and wetted individually by the matrix phase; instead, the fillers are often agglomerates made up of many smaller particles. The degree of dispersion, the strength of the agglomerates and the orientation of the particles can all be important in determining the mechanical and physical properties of the composite material. Ahmed and Jones (1990) pointed out that agglomerates tend to contain voids and air spaces so that their apparent volume is considerably greater than the true volume of the filler material. If the agglomerates are hard and have appreciable mechanical strength so that they are not easily broken up, the filled material can have a modulus greater than expected from the weight of material used as the filler because the volume of the aggregates is larger than the true volume of the filler particles. Soft, easily disintegrated aggregates, on the other hand, would be expected to give the opposite effect.
Although there is no valid general theory for the stress-strain behavior of filled systems, it is known from observations that generally fillers cause a large decrease in elongation-to-break and also often decrease the tensile strength of a material (compared with the matrix). Because of the large stresses and strains encountered during tensile tests, debonding is often observed. Debonding is the result of creating voids due to poor interfacial adhesion or due to the breaking up of agglomerates of low strength. Tensile strength and modulus drastically decrease after debonding takes place.

In a related investigation, Sjögren and Berglund (1997) examined the effect of glass beads on the stress-strain behavior of isotactic polypropylene. They observed that debonding between polypropylene and glass beads initiated at about 0.7% strain and was then followed by plastic yielding of the matrix at the debonded sites. During deformation to ultimate failure, material stiffness is significantly reduced. This is partly because of strain softening of the matrix and partly because of damage associated with debonded cracks. The maximum stress and strain-to-failure decreased with increasing glass diameter. For the smaller beads, the matrix failed in a ductile tearing process. With the larger diameter beads, the final matrix fracture occurred through a more brittle crack growth process. Large debonding voids were formed at high strains. A likely mechanism for the final fracture with large glass beads is the linking of debonded voids by crack growth perpendicular to the load direction. A few large debonded voids formed with large particles are apparently more detrimental than many small debonded voids. Finally, impact strength was observed to directly correlate with the ability of the material to reach high strain to failure in a quasi-static tensile test.
Previous studies by Pukánszky (1990) have investigated the composition dependence of yield stress for PVC/CaCO$_3$ composites. Two different CaCO$_3$ fillers were used with average particle diameters of 3.6 and 58 µm. Composite yield stress decreases with increasing filler content in both cases, indicating that debonding is the dominant deformation mechanism. Debonding occurs before reaching the yield stress of the polymer; most of the load is carried by the matrix. Similar correlations are also observed in polypropylene (PP)/CaCO$_3$ composites (Pukánszky, et al. 1994). A different composition dependence is observed in a low density polyethylene matrix when the filler with the smaller particle size is added. The yield stress of the composite increases monotonically with increasing filler content, i.e. the filler carries a part of the external load. Yield stresses which exceed that of the neat polymer indicate the presence of larger than average stresses around the inclusions and possibly the formation of a hard interlayer with increased modulus and yield stress. If the particle size is large, the load carried by the filler is always smaller than the matrix yield stress, i.e. debonding stress is less than yield stress, hence debonding takes place and the composite yield stress continuously decreases with increasing filler content. When the specific surface area of the filler is larger (smaller particles), the load carried by the filler can significantly exceed the yield stress of the matrix.

In conclusion, strong adhesion leads to matrix yielding, while decreased interaction leads to debonding, with corresponding dependence of composite yield stress on filler content. Debonding starts at the pole of the particles and proceeds catastrophically towards the equator if the elastic deformation energy of the matrix is sufficient for the creation of new surfaces. The strength of the interaction, the size of the
particles and the properties of the interphase determine the stress necessary to separate the matrix/filler interface. The thickness of the interphase depends on the strength of the interaction, and there was found to be a linear correlation between the size of the interlayer and the reversible work of adhesion.

2.1.2 Failure Mechanisms of Particulate Composites

Homogeneous material consisting of a single constituent usually presents straightforward failure modes under different loading and boundary conditions. In contrast, composites demonstrate a variety of failure modes. This is because of the complexity of interactions between the matrix and the filler in a composite structure. Phenomena such as plastic yielding, cavitation (the appearance of voids) and interfacial debonding (adhesive failure between the matrix and filler particles) lead to gross non-linearities in stress-strain behavior of polymeric composites.

In composites filled with rigid particles, the critical stress intensity and fracture energy increase with the addition of the filler, at least for lower volume fractions. The most generally accepted explanation for this behavior, using the analogy of a dislocation moving through a crystal, is that a crack in a body possesses "line tension" and that when it meets an impenetrable array of obstacles, it becomes pinned. In order to move past the obstacles, the crack would have to bow. This leads to an increase in fracture energy. The fracture energy reaches a maximum at a critical filler volume fraction and then decreases with the further addition of particles, which implies that there may be another mechanism that competes with the crack front pinning at higher filler volume fractions.
In polymer composites filled with soft particles, the toughness of the glassy polymers (e.g. epoxy resin) increases with the addition of filler particles. This is believed to be because of the wide spread presence of energy absorbing deformation processes such as crazing and shear yielding. Both shear yielding and crazing involve localized or nonhomogeneous plastic deformation of the material arising from strain softening and from geometric factors. The main difference between these mechanisms is that shear yielding occurs at constant volume, whereas crazing involves an increase in the volume of the composite.

Addition of rigid particles of varying stiffness, surface properties and geometry to polymer matrices of different properties results in different failure behavior. Parameters that affect this type of failure include particle size, filler concentration, filler surface treatment, matrix and filler properties, superimposed pressure, and the rate of strain. It is well established that the fracture of particulate composites is associated with interfacial debonding between the matrix and particles, particle cracking, and the ductile plastic failure in the matrix depending on the relative stiffness and strength of the two constituent materials and the interface strength. If both constituent materials have material properties of the same order of magnitude or if the strength of particle is low, particle cracking can occur. On the other hand, if the embedded particles are much stiffer and stronger than the matrix, matrix cracking (or cavity formation) and particle/matrix interface debonding become the major damage modes. However, the importance of interfacial strength in the fracture is not clear. Along with interfacial debonding between the particle and the matrix, composites undergo a variety of damage modes such as fracture of particles and cracking in the matrix, which develop from an early stage of
deformation under the influence of monotonic and cyclic loads. These damage modes affect the important material properties such as tensile strength, fatigue strength and fracture toughness. Therefore, it is important that emphasis should not be placed solely on their reinforcing effect, but also on the influence of damage on mechanical performance of the composite.

A schematic representation of the possible damage modes for a two-phase particulate composite when subjected to remote loading is shown in figure 2.1 (Ravichandran and Liu, 1995), where the particles are assumed spherical in shape. Upon loading at a critical strain level, the interfacial bond may break and the adhesion is no longer perfect. The polymer will then deform more than the filler so that elliptical cavities or voids develop around each filler particle called debonding as shown in figure 2.1(B) and/or by cavity formation for well bonded particles as shown in figure 2.1(C). Debonding is the result of creating voids during the stretching of a specimen due to poor interfacial adhesion and, consequently, of volume growth during loading.
Figure 2.1 Schematic of particulate composites subjected to uniaxial tension: (A) undamaged; (B) damaged by debonding at the apex; (C) damaged by cavity formation (Ravichandran and Liu, 1995)

Tensile strength and modulus drastically decrease after debonding takes place, and there is a large increase in volume (dilation) as elongation continues. Such a phenomenon has been studied by Ravichandran and Liu (1995), Kwon, Lee and Liu (1997, 1998). These studies investigated the nonlinear constitutive response of a damaged particulate composite in terms of the change in volume dilation and showed that the stress-strain response is nearly linear when there is little or no volume dilatation and the non-linearity sets in once the dilatation becomes significant. The particulate composites of interest (polymeric, rubber) are nearly incompressible prior to any damage and the damage in the material due to deformation is manifested in the form of volume dilatation. A typical uniaxial stress-strain curve and the corresponding volume dilation for an elastic particulate composite are shown in figure 2.2 (Ravichandran and Liu, 1995). The usual
assumption made regarding the damage process in particulate composites is that the maximum strain (or a measure of it) attained by the materials during their deformation history controls the constitutive response.

Figure 2.2 Uniaxial stress-strain response and dilation as a function of strain

(Ravichandran and Liu, 1995)

An earlier experimental study of uniaxial deformation of particle-filled polyolefin revealed two different modes of phase decohesion as shown in figure 2.3 (Oshmyan and Muravin, 1997). At low filler fraction as shown in figure 2.3(A), the microhomogeneous mechanism takes place when the interparticle interactions may be neglected. It is characterized by complete uncorrelated debonding before yielding and a similarity of further deformation in the vicinities of different particles. Above certain filler content (about volume fraction 20%), when interparticle interactions are noticeable, a
microhomogeneous mechanism is changed to a craze-like process of which the characteristic features are correlated debonding in narrow zones, transverse to the loading direction, and concentration of further deformation mostly inside these microporous regions as shown in figure 2.3(B). Formation of the microporous zones in the process of correlated debonding screens decohesion of the remaining particles in their neighborhood. As the concentration of filler increases, the elongation at which debonding takes place decrease. The debonding mechanism is very important for further plastic deformation and fracture. It determines ductile or brittle fracture, macro homogeneous flow or deformation with necking.

The mechanism of microdamaging may be thought of as a phenomenon passing through two different stages of damage; the first being the adhesive debonding of the
matrix from the filler and the second being the fracture of the matrix (Moshev and Evlampieva, 1997). Clearly, the debonding diminishes the resistance of the structural element. However, the latter retains a capability to resist the extension for some time, although at a lower modulus. Only after the matrix part of the element has been broken, may one consider that resistance has vanished.

Most of the research regarding particulate composites assumes perfect adhesion between the filler and the polymer matrix, as well as perfect dispersion of the individual filler particles. Perfect adhesion means that there is no relative movement of the two phases across the interface up to loads equal to the one being considered. In many practical applications, the individual fillers are not separated from one another and wetted individually by the matrix phase; instead, the fillers are often agglomerates made up of many smaller particles. The degree of dispersion, the strength of the agglomerates and the orientation of the particles can all be important in determining the mechanical and physical properties of the composite material. These important factors are often difficult to measure experimentally. Thus, it is not surprising that there is a lot of scatter in experimental data on particulate composites, and the agreement between theory and experiment is often not very good.

2.1.3 Residual Stresses in Particulate Composites

The first stage in the manufacture of polymeric products involves the mixing all necessary chemical constituents, i.e. monomer, fillers, pigments, initiator, cross-linking agents, etc, followed by polymerization. The resultant chemically structured material then needs to be fashioned into the desired shape via a suitable processing operation such as
casting and molding. Generally these thermal processing techniques produce important side effects that considerably affect the performance of acrylic particulate composites. Polymeric materials are viscoplastic materials – their response to mechanical and thermal loads is time-dependent. At higher temperatures, this time-dependence is more pronounced, and at lower temperatures the response is predominantly elastoplastic. During thermal processing, viscoplastic properties change continuously with changing temperature, with the most pronounced changes occurring around the glass transition temperature $T_g$. At this temperature, the material solidifies, freezing in a majority of the strains within the material, and thus resulting in the presence of residual stress after processing. Non-uniform solidification plays a key role in the induction of residual stress within polymeric products. Throughout the processing, the material is subjected to non-uniform temperature distributions and thermal expansions, which result in stress in the material. Due to the low modulus in the softened state, the material can hardly sustain any of the deviatoric stresses that arise from the thermal expansions. A majority of these deviatoric stresses tend to vanish from the system, despite the presence of temperature distributions. The temperature distribution is eventually removed from the system, but only after solidification is complete. The resistance of the material to any removal of the "remaining" temperature gradients while in the solid state thus induces residual stresses in the system, which could result in distortion and asymmetry in the final product.

It is shown that most of the residual stresses are induced in the cooling zone during nonuniform solidification (Tropsa et al., 2000). In the cooling zone, surface temperatures decrease very quickly to below the $T_g$ of the material, thus creating a solid layer around the plate surfaces. Solidified material can sustain mechanical strains, and
considerable stresses can be generated. The interior of the plate is still soft and no major stresses are induced at this stage. These two distinguished regions, solidified and softened, are separated by a solidification front, which gradually moves towards the plate interior as cooling progresses. The plate is solid when the temperature throughout the plate has fallen below the $T_g$ of the material. At this stage, substantial temperature gradients still exist across the plate, with the plate interior remaining warm with temperatures close to $T_g$, while the plate edges have almost reached the cooling temperature. At the end of the cooling zone, temperature gradients have largely disappeared from the plate, leaving thermal stresses induced via the coefficient of thermal expansion. Nonuniform thermal contractions are responsible for most of the residual stress in the material at a uniform temperature. In the final stages of cooling, the interior of the plate tends to contract more than the surface layers, which prevent the full contraction of the inner region. As a result, the inner region is stretched into a state of permanent compression.

Due to the heterogeneous nature of composites and the different and sometimes very dissimilar expansion/contraction behavior and mechanical properties of the constituents, thermal stresses are easily generated and can prove troublesome. It is well known that within the particulate composite microstructure, there exists microstressed associated with the CTE mismatch between the matrix and the particle. For the composite prepared using lightly cross-linked poly-methyl methacrylate (PMMA) filled with alumina trihydrate (ATH), these microstresses can be imaged using the fact that PMMA is stress optically birefringent. The microstresses imaged using this technique are indeed due to CTE mismatch, since they dissipate at temperatures close to the $T_g$ of the PMMA.
(as shown in figure 2.4). These stresses can be quantified by calculation or by direct measurement and are of the order of between 15% and 75% of the tensile strength of the composites. Therefore the thermal stress associated with the CTE mismatch between the matrix and the particle is an important factor for the failure of particulate composites subjected to thermomechanical loads. These thermal effects are exacerbated by thermal cycling, which can occur in a working environment. Thermal cycling involves repeatedly cycling a specimen or material between two temperatures with a sufficient dwelling time at either extreme to allow thermal equilibrium to be attained. It is assumed that the cooling (or heating) rate is not fast enough to induce thermal shock which is perhaps, best defined as the presence of a larger thermal gradient through the specimen. Plunging an unprotected specimen at ambient temperature into liquid nitrogen is an example of how thermal shock can be produced.
Asp et al. (1997) used finite element analysis to investigate the effect of glass bead content and residual stresses on the failure initiation in isotactic polypropylene composites for the cases of interfacial debonding, plastic yielding and cavitation. They compared the initial stress-strain behavior of polypropylene and polypropylene composites with 20% glass beads, and discovered that both maximum stress and global strain for yield initiation decrease with the introduction of glass beads. The initiation of substantial nonlinear behavior exhibited by the composite, which differed from that of the
matrix material, meant that one of the following three damage mechanisms was likely: plastic yielding of the matrix, cavitation in the matrix or interfacial debonding between polypropylene and the glass beads. Asp et al. considered plastic yielding and then cavitation in their investigation of the likely mechanisms for the initiation of failure in particulate composites. Fu et al. (1992, 1993) considered cavitation as a mechanism of failure initiation in particulate composites. However, the results did not agree with either of the consideration. Residual thermal stresses were demonstrated to have a large effect on the global failure initiation stress. Cavitation always occurs at a higher stress than debonding, and is therefore excluded as a plausible mechanism. Yielding also occurs at a higher global stress than debonding. However, residual stress that is higher than the estimated could lead to yield initiated failure, although experimental data do not support this. Instead, data from the present experimental studies are in support of debonding as the initial failure mechanism.

2.2 Damage Mechanics

Damage is the deterioration of materials, which occurs prior to failure. For centuries failure has been studied as a ‘yes or no’ process related to a critical value of load, stress, strain, and time or number of cycles of loading. 1958 is the year to be considered the starting point of continuum damage mechanics, when Kachanov (1958) published the first paper on a field variable $\psi$ called “continuity”.

In general, a theoretical description of damage mechanics can be rather complicated. Lemaitre (1992) explains the concept of damage in the following way: “The damage of materials is the progressive physical process by which they break. Damage
mechanics is the study, through mechanical variables, of the mechanisms involved in this deterioration when the materials are subjected to loading. At the microscale level, this is the accumulation of microstresses in the neighborhood of defect or interfaces and the breaking of bonds, which both damage the material. At the mesoscale level of the representative volume element (RVE), this is the growth and the coalescence of microcracks or microvoids which together initiate one crack. At the macroscale level, this is the growth of that crack. The two first stages may be studied by means of damage variables of the mechanics of continuous media defined at the mesoscale level. The third stage is usually studied using fracture mechanics with variables defined at the macroscale level”.

2.2.1 Types of Damage

Even if the damage at the microscale is governed by one general mechanism of debonding, at the mesoscale it can manifest itself in various ways depending upon the nature of the materials, the type of loading and the temperature. Types of damage are summarized according the work of Kachanov (1986).

(1) Creep damage

When a metal is loaded at certain elevated temperatures, the plastic strain involves viscosity. When the strain is large enough, there are intergranular decohesions that produce damage and an increase of the strain rate through the period of tertiary creep. As for ductile damage, the gradients of creep damage are similar to the viscoplastic strain gradients.
(2) Ductile plastic damage

The damage is called ductile when it occurs simultaneously with plastic deformations larger than a certain threshold. It results from the nucleation of cavities due to decohesions between inclusions and the matrix followed by their growth and coalescence through the phenomenon of plastic instability. As a consequence, the degree of localization of ductile damage is comparable to that of plastic strain.

(3) Brittle damage

On the other hand, the damage is called brittle when a crack is initiated at the mesoscale without a large amount of plastic strain. This means that the cleavage forces are below the forces that could produce slips but are higher than the debonding forces.

(4) Fatigue damage

Under the action of cyclic loading, a gradual deterioration of the structure of a material, caused by the accumulation and growth of micro and macro cracks, takes place. When a material is subjected to a cyclic loading at high values of stress or strain, damage develops together with cyclic plastic strain after a period of incubation preceding the phases of nucleation and propagation of microcracks. The degree of damage localization is higher than that for ductile or creep damage. If the material is strain loaded, the damage induces a drop of the stress amplitude.

(5) Chemomechanical damage

Under the action of a tensile stress (especially the cyclic one) metals operating in aggressive media (for example, in sea water) are subjected to intensive corrosion ("stress corrosion") or to some other chemical reaction.
(6) Environmental degradation

Some materials (geo-materials, polymers) change their mechanical properties under the influence of the environment even in the absence of stress.

2.2.2 Measurements of Damage

There are many ways to characterize the material degradation experimentally. According to the works of Lemaitre (1996), the methods of measuring the damage in materials are summarized as follows.

(1) Direct measurement

The direct measurement consists of the evaluation of the total crack areas lying on a surface at mesoscale. And this can be done by observing micrograph pictures.

(2) Degradation of elastic modulus

This is a nondirect measurement based on the influence of damage on elasticity. It assumes uniform homogeneous damage in the specimen gauge section. If $\overline{E} = E(1 − D)$ is considered as the effective elasticity modulus of the damaged material, the values of the damage may be derived from measurements of $\overline{E}$, provided that the virgin Young's modulus $E$ is known:

$$D = 1 − \frac{\overline{E}}{E}$$  \hspace{1cm} (2.1)

This very useful method requires accurate strain measurements. $\overline{E}$ is most accurately measured during unloading.
(3) Ultrasonic waves propagation

Another technique for evaluating damage based on the variation of the elastic modulus consists in measuring the speed of ultrasonic waves. For frequencies higher than 200 kHz, the damage is calculated by:

$$D = 1 - \frac{V_L^2}{v_L^2}$$

(2.2)

where $v_L$ is the longitudinal wave speed in the original material, $\bar{v}_L$ is the longitudinal wave speed of a damaged material.

(4) Variation of microhardness

This is another nondirect measurement based on the influence of damage on the plasticity-yield criterion through the kinetic coupling. The damage can be defined as

$$D = 1 - \frac{H}{H^*}$$

(2.3)

where $H$ is the microhardness after certain number of load cycles, $H^*$ is the microhardness of the material without any damage. It is also a convenient way to evaluate damage fields because the microhardness can be measured easily using a Nano Indenter test.

(5) Variation of density

In the case of pure ductile damage, the defects are cavities that can be assumed to be roughly spherical, which means that the volume increases with damage. Let $\bar{\rho}$ be density associated with the damaged state and $\rho$ be the density of the initial state; it is easy to derive the following relationships between the damage $D$ and the variation of the density as:
\[ D = \frac{\delta S_D}{\delta S} = \left(1 - \frac{\bar{\rho}}{\rho} \right)^2 \]  

(2.4)

(6) Variation of electrical resistance

The effective intensity of the electrical current can be defined in the same way as the effective stress was defined. If the same current intensity \( i \) is considered for the nondamaged and the damaged elements, the damage \( D \) may be derived from the two expressions

\[ D = 1 - \frac{V}{\bar{V}} \left( \frac{\bar{r}}{r} \right) \]  

(2.5)

where \( V \) is the potential difference for a nondamaged element with resistivity \( r \); and \( \bar{V} \) is the potential difference for damaged element with resistivity \( \bar{r} \).

(7) Variation of cyclic plasticity response

The influence of damage on plasticity may be used to measure the low cycle fatigue damage. Considering a test at constant plastic strain amplitude, if \( \Delta \sigma^* \) is the stress amplitude at stabilization at the end of the cyclic softening or hardening period and before the beginning of the damage process, the damage can be defined as

\[ D = 1 - \frac{\Delta \sigma}{\Delta \sigma^*} \]  

(2.6)

where \( \Delta \sigma \) is the amplitude of stress at stabilization. This method successfully identifies the evolution of damage during low cycle fatigue of metals, except when stabilization of the cyclic softening or hardening does not occur.
(8) Tertiary creep response

Assuming that the damage process begins at the end of secondary creep and let \( \dot{\varepsilon}_p \) be the creep rate during tertiary creep, the damage parameter can be derived to identify creep damage during creep tests,

\[
D = 1 - \left( \frac{\dot{\varepsilon}_p^*}{\dot{\varepsilon}_p} \right)^{\frac{1}{N}}
\]

(2.7)

where \( \dot{\varepsilon}_p^* \) is the minimum creep rate determined by Norton's law of secondary creep; and \( N \) being temperature-dependent material parameters. This method yields good results, which are in accordance with those obtained by measuring the variation of the elasticity modulus.

(9) Acoustic emission

It is a good method for detecting the location of the damaged zone, but the results remain qualitative as far as the values of the variable \( D \) are concerned.

(10) Remaining life

From an engineer’s point of view, the main objective of a damage theory is to allow predictions of the lifetime of a structure. Then the remaining life concept is a natural way to define damage. According to the linear Miner’s rule, where it is assumed that contribution of each cycle is equal, the damage can be defined as

\[
D = 1 - \frac{N}{N_F}
\]

(2.8)

where \( N \) and \( N_F \) represent, respectively, the number of cycles already applied and the total number of cycles to failure.
Cumulative hysteresis dissipation

The area of the hysteresis loop represents the energy dissipation corresponding to one load cycle. With each load cycle, the material absorbs a certain amount of hysteresis dissipation by which the fatigue damage may be characterized. This means that with increasing number of cycles, the fatigue damage accumulates, corresponding to the hysteresis dissipation dissipated, until it reaches a certain critical value at which fatigue failure occurs. The total dissipated energy to failure can be used as a measure for fatigue life prediction.

2.2.3 Cumulative Fatigue Damage

Fatigue damage occurs when a material experiences cyclic or repetitive loading resulting in deterioration or damage in the material microstructure. Therefore, it is possible for failure to occur at the load with the magnitude considerably lower than that under static conditions. Cumulative fatigue damage analysis plays a key role in the life prediction of components and structures subjected to cycling loadings. Since the introduction of damage accumulation concept, the treatment of cumulative fatigue damage has received increasingly more attention. As a result, many fatigue damage models have been developed. Recently, some comprehensive papers have appeared to review the considerable efforts made on cumulative fatigue damage modeling, such as Fatemi and Yang (1998), where the main approaches for lifetime prediction are grouped into six categories: linear damage rules, nonlinear damage curve and two-stage linearization approaches, life curve modification methods, linear elastic fracture mechanics models, continuum damage mechanics models and energy-based theories.
Here a brief review of cumulative fatigue damage theories is presented, emphasizing the approaches of continuum damage mechanics models.

### 2.2.3.1 Fatigue Damage Related Parameters

There are four major quantities to be considered with fatigue damage: loading range, temperature, loading rate, and fatigue damage criteria. Figure 2.7 shows Variables used to define cyclic loading.

The loading range may be the most important parameter to determine the fatigue life. Fatigue life has been characteristically partitioned into a low cycle fatigue (LCF) regime and a high cycle fatigue (HCF) regime. LCF usually represents cycling in a range where irreversible inelasticity is encountered and the inelastic strain is greater than the elastic strain. HCF is cycling at small enough load amplitude, where the elastic strain predominates the material deformation, and the fatigue lives are very long. Strain or deformation controlled loading mode is usually used for LCF testing. The material can be tested at various load levels and the number of cycles to failure is counted. Eventually, enough data are accumulated to plot an endurance curve, or $S - N$ curve, in which fatigue failure load $S$ is plotted versus the number of cycles to failure $N$. The vertical axis is usually a linear scale and the horizontal axis is usually a logarithmic scale. There always exists considerable scatter in fatigue data. It is a consequence of the fatigue sensitivity to a number of test and material parameters that are impossible to control precisely.

Fatigue behavior becomes more complicated at high temperatures than at room temperature because a complex interaction between mechanical and thermally activated...
time-dependent processes may be involved. Therefore, thermal fatigue is more complex than fatigue at room temperature under cyclic mechanical loads because the temperature changes can cause the material properties to change significantly.

Due to the creep effect, for a given strain range, low loading rates will introduce a large amount of time-dependent creep strain that will influence cyclic fatigue behavior. The combined mechanisms of creep and fatigue damage have a more deleterious effect on the mechanical performance of materials than either mechanism acting independently. Creep-fatigue damage is sensitive to the strain rate because creep strain, which builds up in the course of fatigue deformation, is dependent on the strain rate. It has been documented that at high frequencies of cycling, materials exhibit a hardening tendency and reflect a creep-resisting characteristic. On the other hand, at lower frequencies, below some critical value, materials show lower strength and develop larger time-dependent creep strains.

Fatigue life prediction is closely tied to monitoring and analyzing evolving material degradation. Many experimental and theoretical investigations of the fatigue damage process have been conducted in order to construct a reliable fatigue damage criterion that can yield an accurate prediction of the fatigue life. Because of the variability of the fatigue phenomena, the accuracy of the prediction will depend on the understanding of the laws governing fatigue damage, its mechanisms and growth, and to establish the effect of decisive internal and external factors that influence the fatigue life. In practice, a damage criterion is chosen, and its values are correlated with the number of cycles to failure. There are many fatigue damage criteria commonly used, for example,
stress amplitude and mean stress, strain or inelastic strain range, hysteresis dissipation, and load-drop parameter.

2.2.3.2 Linear Elastic Fracture Mechanics (LEFM) Models

The crack growth concepts developed in 1950s and 1960s have enjoyed wide acceptance since cracks are directly related to damage, and since modern technology has provided sophisticated tools and techniques which enable measurement of very small cracks in the order of 1µm. Several macro fatigue crack growth models based on LEFM have been developed to account for the cumulative fatigue damage process. But, when the crack length is physically short, the applicability of fracture mechanics becomes questionable.

Miller (1982, 1987) investigated the behavior of very short cracks and proposed that crack initiation occurs immediately in metal fatigue, and that the fatigue lifetime is composed entirely of crack propagation from an initial defect size. The early two phases were named as microstructurally short cracks and physical small crack growth, which are both elasto-plastic fracture mechanics type cracks. Based on their experimental observations and interpretation, Vasek and Polak (1999) identified two damage regimes. In the crack initiation regime, a constant crack growth rate was proposed described by

\[
\frac{da}{dN} = v_i \quad a_0 \leq a \leq a_c
\]  

(2.9)

and in the crack propagation regime, the dependence of \(da/dN\) on the crack length was approximated by a linear relation:

\[
\frac{da}{dN} = v_i + k(a - a_c) \quad a_c \leq a \leq a_f
\]  

(2.10)
where $v_i$ is the crack growth rate independent of applied cycles, $k$ is a coefficient, and $a_0$, $a_c$ and $a_f$ are the initial, critical and final crack length, respectively. The critical crack length defines the transition from the initiation phase to the propagation phase.

### 2.2.3.3 Continuum Damage Mechanics Models

Theory of damage mechanics has been employed to predict the fatigue behavior because of the shortcomings and the limitations of the conventional fatigue damage analyses. The damage mechanics theory introduces a set of macroscopic internal state variables to describe the evolution of inherent micro-cracks and voids in the form of material degradation or damage. Chaboche (1988) argued the importance of continuum damage mechanics. Fatigue damage is a form of material degradation caused by the initiation, growth and coalescence of micro-cracks in a material element due to cyclic loading and is therefore ideally suited to be characterized by the theory of damage mechanics. This approach is developed based on the original concepts of Kachanov (1958) in treating creep damage problems. The successful application of continuum damage mechanics in modeling the creep damage process has encouraged many researches to extend this approach to ductile plastic damage, brittle fracture and fatigue damage. Continuum damage mechanics can also be applied to composites and concrete materials. But the continuum damage models are mainly developed for uniaxial fatigue loading. Some difficulties arise when these models are extended to multiaxial loading.

Based on the continuum damage mechanics concept, many forms of fatigue damage equations have been developed after Chaboche's work. Such models include those proposed by Lemaitre and Chaboche (1990), Lemaitre and Plumtree (1979), Wang
(1992), Wang and Luo (1990), Chow and Chen (1992), Basaran and Yan (1998), Basaran and Tang (2002), Basaran and Nie (2004). Most damage mechanics based approaches are very similar to Chaboche's model in both form and nature. The main differences lie in the number and the characteristics of parameters used, in the requirements for additional experiments, and in their applicability. A damage potential function is the common feature defining the damage potential. On the other hand, the damage mechanics theory proposed by Basaran and co-worker does not use a damage potential function and entropy is used as the primary damage metric.

2.2.3.4 Energy Based Approach

The area of the hysteresis loop represents the energy dissipation corresponding to one load cycle. With each load cycle, the material absorbs a certain amount of hysteresis dissipation by which the fatigue damage may be characterized. This means that with the increasing number of cycles, the fatigue damage accumulates, corresponding to the hysteresis dissipation, until it reaches a certain critical value at which fatigue failure occurs. Because of the connection between hysteresis dissipation and the fatigue behavior, many studies have been carried out on the energy method. It has been realized that an energy-based damage parameter can unify the damage caused by different types of loading such as thermal cycling, creep and fatigue. Energy-based models can also include mean stress and multiaxial loads since multiaxial fatigue parameters based on strain energy have been developed. In fact, some part of the energy imparted goes into heat, and a portion of hysteresis dissipation consumed during each cycle contributes to the damage in material.
Kujawski and Ellyin (1984) developed a preliminary damage model by using plastic strain energy density as a parameter. It was later found that some inefficiencies were associated with the plastic strain energy density approach. For example, the effect of mean stress cannot be directly incorporated in the determination of the hysteresis dissipation. Leis (1988) proposed an energy-based nonlinear history-dependent damage model which links the damage parameter to fatigue life. By examining constant strain amplitude test data, Niu (1987) found out that the cyclic strain hardening coefficient changes during the cycling process, while the cyclic strain hardening exponent had a negligible change. The fatigue damage function was constructed in terms of fraction of the plastic strain energy.

2.3 Micromechanics of Particulate Composites

The application and estimation of the effective mechanical properties of random heterogeneous multiphase materials are of great interest to researchers and engineers in many science and engineering disciplines. There are many different methods and tools that can be used to deliver the macroscopic constitutive response of heterogeneous materials from a local description of the microstructural behavior. In the development of the homogenization procedures for heterogeneous materials, we have to define both the homogenization step itself (from local variables to overall ones) and the often more complicated localization step (from overall controlled quantities to the corresponding local ones). Numerous papers on the determination of effective thermomechanical properties of heterogeneous materials have been published. However, up to now no
formula has been derived which is theoretically well founded and fits experimental results for the whole range of volume concentrations.

The first school employs variational principles to obtain mathematical lower and upper bounds for effective properties of multiphase particulate composites. At that level, we can mention classical Hashin-Shtrikman bounds (1963), Walpole’s bounds (1966), and Willi’s bounds (1991) in the linear context, and more recent works give pertinent results for the inelastic behavior.

The second school is well known as the effective medium approach based on generalizations of the Eshelby method (1957), which includes the self-consistent method and the Mori-Tanaka method (1973). These techniques are particularly useful for situations with random microstructures. Generally they deliver only average local stress and strains (ensemble averages on a given kind of particle or grain orientation) and are not formulated in order to obtain the local stress (or strain) fields, taking into account particle to particle interactions.

The third school aims at direct determination of effective properties of composites with randomly located particles by introducing some approximations or by assuming certain special configurations for particles dispersing in matrix materials. For example, effective elastic properties of two-phase composites can be evaluated by a power series in particle volume fraction $\phi$, with each $\phi^n$ term corresponding to averaged $n$ particle interaction effects.

The fourth school assumes numerical techniques, most often based on the assumption of microstructure periodicity, and several analytical results were obtained. For example, solutions for single coated particles with suitably reduced moduli of the
elastic interphase or solutions for spring-type interface, provide fairly simple analytical forms of local stresses as functions of the phase moduli, interface or interphase properties and remotely applied stresses. In these cases, which may be quite particular, the periodic homogenization techniques are able to describe local stress (and strain) fields and their evolutions very correctly. They also deliver the overall stress strain behavior of the considered representative volume element of material. Practically, one uses finite element methods or fast Fourier transform solutions. These numerical methods are limited to the quasi-periodic situations. Moreover their cost is really high and their direct use inside a true structural analysis is presently limited to very special cases. Here also, these methods do not really get the status of constitutive equations (they are usable only through a step by step analysis).

Based on generalizations of the Eshelby method (Eshelby, 1957), a novel micromechanical framework has been proposed by Ju and Chen (1994a, 1994b) to investigate the effective mechanical properties of elastic multiphase composites containing many randomly dispersed ellipsoidal inhomogeneities with perfect bonding. Within the context of the representative volume element (REV), four governing micromechanical ensemble-volume averaged field equations are presented to relate ensemble-volume averaged stresses, strains, volume fractions, eigenstrains, particle shapes and orientations, and elastic properties of constituent phases of linear elastic particulate composites. Then various micromechanical models can be developed based on the proposed ensemble-volume averaged constitutive equations. In Ju and Tseng (1996), a formulation combining a micromechanical interaction approach and the continuum plasticity is proposed to predict effective elastoplastic behavior of two-phase particulate
composites containing many randomly dispersed elastic spherical inhomogeneities. Explicit pairwise interparticle interactions are considered in both the elastic and plastic responses. Furthermore, the ensemble-volume averaging procedure is employed and the formulation is of complete second order.

It is well known that interface imperfections can significantly affect the mechanical properties and failure mechanisms as well as the strength of particulate composites. The nature of the bond between particles and the matrix material has a significant affect on the mechanical behavior of particulate composites. Most analytical and numerical models assume that the bond between the filler and matrix is perfect and can be modeled using the continuity of tractions and displacements across a discrete interface. When the perfect interface conditions are present, the primary result is the well-known Eshelby’s (1957) solution of the ellipsoidal inclusion problem. However, internal defects and imperfect interfaces are well known to exist in composites and the incorporation of such phenomena into the general theory requires modification and relaxation of the continuity of displacements between the constituents. Rather than having perfect interface, the imperfect interface bond may be due to the very compliant interfacial layer known as interphase or interface damage. Such an interfacial zone may have been created deliberately by coating the particles. It may also develop during the manufacturing process due to chemical reactions between the contacting particles and matrix material or due to interface damage from cyclic loading. Moreover the strength of the bond at the interface controls the mechanical response and fatigue life of the composite, (Basaran, Nie and Hutchins, 2004). By controlling the stress-strain response of the interphase, it is possible to control overall behavior of the composite.
Clearly the interface imperfections can significantly affect the mechanical properties and failure mechanisms as well as the strength of the particulate composites. The influence of an interfacial zone on composite mechanical and thermal behavior has already been investigated by a number of authors, such as Benveniste (1985), Achenbach and Zhu (1989, 1990), and Hashin (1990, 1991). There have also been several investigations in the literature that concentrate on the effect of imperfect interfaces in composites, which may be appropriate in the case of thin coatings on inclusions. In related studies, two analytical models have been proposed. First is the spring layer model, which involves a very thin interfacial zone of unspecified thickness (Benveniste 1985; Achenbach and Zhu 1989, 1990 and Hashin 1990, 1991). In this model it is assumed that the radial and the tangential tractions are continuous across the interphase for reasons of equilibrium, but because of the presence of the interphase, the displacements may be discontinuous from the filler particle to the matrix. The model assumes that the tractions are proportional to the corresponding displacement discontinuities. The proportionality constants therefore characterize the stiffness and strength of the interphase.

Figure 2.5 Spring layer model (Hashin, 1991)
Suppose that two different homogeneous media, labeled 1 and 2, are joined by an imperfect interface as shown in figure 2.5. With respect to a local orthogonal system, the following relations describe the imperfect interface (Hashin 1991):

\[
T_n^{(1)} = T_n^{(2)} = D_n [u_n], \quad [u_n] = u_n^{(1)} - u_n^{(2)} \tag{2.11}
\]

\[
T_s^{(1)} = T_s^{(2)} = D_s [u_s], \quad [u_s] = u_s^{(1)} - u_s^{(2)} \tag{2.12}
\]

\[
T_t^{(1)} = T_t^{(2)} = D_t [u_t], \quad [u_t] = u_t^{(1)} - u_t^{(2)} \tag{2.13}
\]

where \( n \) is the normal direction and \( s, t \) are the tangent directions. \( D_n, D_s, \) and \( D_t \) are the spring constant type interface parameters. Infinite values of these parameters imply that there are no interface displacement jumps and the perfectly bonded interface conditions exist. At the other extreme, zero values of \( D_n, D_s, \) and \( D_t \) imply that the interface tractions do not exist and the filler is debonded from the adjoining matrix media. Finite positive values for the interface parameters define an imperfect interface, which lies between two extreme cases mentioned above.

In many particulate composites, a thin layer of some other elastic phase intervenes between a particle and the matrix. The imperfect interface bond may be due to the compliant thin interfacial layer that is assumed to have perfect boundary conditions with the matrix and the particle. A considerable amount of the literature is concerned with the related problem of dealing with composites with coated reinforcement where such materials are viewed as three phase composites. So the alternative model described the interphase as a layer between particles and matrix of a specified thickness and of elastic constants different from those of the matrix and the particles (Benveniste 1985; Achenbach and Zhu 1989, 1990 and Hashin 1990). The literature shows that a thin, flexible interphase layer is equivalent to the above spring layer model for the imperfect
interface and the interface parameters have been determined in terms of the interphase properties and the thickness (Hashin, 1991). The effect of the coating, when it is thin, can be conveniently expressed in terms of the imperfect interface so that only two phases remain. It is indeed possible, as shown in Hashin (1990, 1991), to express imperfect interface parameters simply and directly in terms of the interphase (coating) characteristics.

It is expected that the interface parameters will be different in tension and compression. Such an effect is easily incorporated into the effective bulk modulus and thermal expansion coefficient analysis. It will change the bulk moduli for isotropic tension and compression, as well as the thermal expansion coefficients for heating and cooling. The sign of the radial interphase stress can determine the choice among the different interface parameters. But this presents a rather difficult problem in which there are different interface regions defined by tensile and compressive normal tractions and their boundaries are \textit{a priori} unknown.

As a related matter, it should be mentioned that if the elasticity problem with interface conditions is regarded in a mathematical fashion without reference to the physical situation it describes, there arises the following difficulty: the normal displacement continuity cannot be negative for this since it would imply penetration of the matrix into the inclusion. The mathematical remedy for this problem would be to require perfectly normal bonding when the normal traction is compressive and imperfect bonding for the case of tension. This would complicate the problem enormously. But, if there is a compliant thin interphase, then the normal displacement discontinuities are defined by the normal deformation of this interphase, which can take place both
outwardly and inwardly. The interphase contribution is approximated by an imperfect interface condition. This approximation assumes that the interface between the matrix and the inclusion interface can be moved inward by a small distance equal to the interphase thickness.

Ghassemieh et al. (2001) developed a flexible and robust finite element model for the micromechanical analysis of the behavior of polymer composites. The model was applied to simulate the stress distribution in particulate filled composites, and its predictions were compared with the available experimental data and with results obtained using other methods reported in the literature. The comparisons were able to show the general accuracy of the developed model. After assessing and validating the model, its simulations were used to evaluate failure modes and the strength of both the rigid and the soft particle filled polymer composites. Epoxy resin filled with glass is taken as an example of a polymer composite filled with rigid particles, while epoxy resin filled with rubber is taken as an example of a polymer composite embedded with soft particles. The predicted position of the maximum direct stress (i.e. the stress in the direction of the applied load) in the glass filled epoxy composite under the described boundary conditions is above the pole of the spherical filler. For a well-bonded sphere, at low volume fractions, cracking starts above the pole and propagates towards the resin matrix in the direction of the direct stress. Results indicate that as the filler volume fraction increases, the location of the maximum direct stress moves further away from the pole. Therefore, as expected, the extent of resin damage and the probability of failure increase when the filler volume fraction is so low that there are no spheres present in the fracture surface. It was also shown that at a particular location on the filler/matrix interface, the normal
stress is zero for the entire range of filler volume fractions examined. Between the equator of the spherical filler and this point the radial/normal stress is compressive. When the maximum, radial stress at the pole exceeds the adhesion forces, interfacial debonding starts and gradually progresses towards the equator. However, because of the compressive nature of the interfacial forces beyond the point of zero normal stress, the propagation of debonding stops.

Vörös et al. (1997) used an energy analysis to show that the relationship between the yield stress of the matrix and the debonding stress determines the mechanism of deformation. In heterogeneous polymer systems, interaction of the components leads to the development of an interphase, which has properties different from those of both components (Morales and White, 1988; Vollenberg and Heikens, 1989). Larger yield stresses than that of the matrix can be achieved with fillers having high specific surface areas leading to the formation of a considerable interphase. Besides the elastic properties, the yield stress of the interphase also changes continuously from the surface of the particles to the matrix. In the absence of debonding, the development of this hard interface leads to increased composite yield stress.
3.1 Introduction

The science of thermodynamics, which began by treating the relations among heat, work and the properties of the systems in equilibrium, has developed into a very general science of energetics for all types of systems: mechanical, chemical and electrical, whether in equilibrium or not. (Groot and Mazur, 1962; Yourgrau et al., 1966; Haase, 1968; Germain, 1986; Ericksen, 1998). Irreversible thermodynamics provides a general framework for the macroscopic description of irreversible processes. In irreversible thermodynamics the so-called balance equation for the entropy plays a central role. This equation expresses the fact that the entropy of a volume element changes with time for two reasons. First it changes because entropy flows into the volume element, second it change because there is an entropy source due to irreversible phenomena inside the volume element. The entropy source is always a non-negative quantity, since entropy can only be created, never destroyed. For reversible transformations the entropy source vanishes. Entropy is a measure of how much energy is unavailable for work.

Entropy is the measure of how much energy or heat is unavailable for work. Imagine an isolated system with some hot objects and some cold objects. Work can be done as heat is transferred from the hot to the cooler objects; however, once this transfer...
has occurred, it is impossible to extract additional work from them alone. Energy is always conserved, but when all objects have the same temperature, the energy is no longer available for conversion into work.

The entropy of the universe increases or remains constant in all natural processes. It is possible to find a system for which entropy decreases but only due to a net increase in a related system. For example, the originally hot objects and cooler objects reaching thermal equilibrium in an isolated system may be separated, and some of them put in a refrigerator. The objects would again have different temperatures after a period of time, but now the system of the refrigerator would have to be included in the analysis of the complete system. No net decrease in entropy of all the related system occurs. This is yet another way of stating the second law of thermodynamics (DeHoff, 1993).

The concept of entropy has far-reaching implications that tie the order of our universe to probability and statistics. Imagine a new deck of cards in order by suits, with each unit in numerical order. As the deck is shuffled, no one would expect the original order to return. There is a probability that the randomized order of the shuffled deck would return to the original format, but it is exceedingly small. An ice cube melts, and the molecules in the liquid form have less order than in the frozen form. An infinitesimally small probability exists that all of the slower moving molecules will aggregate in one space so that the ice cube will reform from the pool of water. The entropy, or disorder, of the universe increases as hot bodies cool and cold bodies warm. Eventually, the entire universe will be at the same temperature so the energy will be no longer usable (DeHoff, 1993).
To relate the entropy source explicitly to the various irreversible processes that occur in a system, one needs the macroscopic conservation laws of mass, momentum and energy in local, i.e. differential form. These conservation laws contain a number of quantities such as the diffusion flows, the heat flow and the stress tensor, which are related to the transport of mass, energy and momentum. The entropy source may then be calculated by using the thermodynamics Gibbs relation, which connects the rate of the change in entropy in the medium to the rate of the change in energy and work. “It turns out that the entropy source has a very simple appearance: it is a sum of terms each being a product of a flux characterizing an irreversible process, and a quantity called thermodynamic force which is related to the non-uniformity of the system”(Groot and Mazur, 1962). The entropy source strength can thus serve as a basis for the systematic description of the irreversible processes occurring in a system.

“As yet the set of conservation laws, together with the entropy balance equation and the equations of state are to a certain extent empty, since this set of equations contain the irreversible fluxes as unknown parameters and can therefore not be solved with the given initial and boundary conditions for the state of the system”(Groot and Mazur, 1962). At this point we must therefore supplement the equations by an additional set of phenomenological relationships, which relate the irreversible fluxes and the thermodynamic forces appearing in the entropy source strength. Irreversible thermodynamics, in its present form, is mainly restricted to the study of the linear relationship between the fluxes and the thermodynamic forces as well as possible cross-effects between various phenomena. This is not a very serious restriction however, since even rather extreme physical situations are still described by linear laws.
“Together with the phenomenological equations, the original set of conservation laws may be said to be complete in the sense that one now has a consistent set of partial differential equations for the state parameters of a material system, which may be solved with the proper initial and boundary conditions” (Groot and Mazur, 1962).

3.2 Conservation Laws

Thermodynamics is based on two fundamental laws: the first law of thermodynamics or the law of conservation of energy, and the second law of thermodynamics or the entropy law. A systematic macroscopic scheme for the description of irreversible processes must also be built upon these two laws. However, it is necessary to formulate these laws in a suitable way. Since we wish to develop a theory applicable to systems of which the properties are continuous functions of space coordinates and time, we shall give a local formulation of the law of conservation of energy. As the local momentum and mass densities may change in time, we will also need local formulations of the laws of conservation of momentum and mass. For the general purposes in solid mechanics, the thermodynamic system will usually be chosen as a given collection of continuous matter, i.e., the system is a closed system not interchanging matter with its surroundings; the bounding surface of the system in general moves with the flow of matter.

3.2.1 Conservation of Mass

Consider an arbitrary volume $V$ fixed in space, bounded by surface $\Omega$. The rate of change of the mass within the volume $V$ is (Malvern, 1969):
\[
\frac{d}{dt} \int_V \rho dV = \int_V \frac{\partial \rho}{\partial t} dV \tag{3.1}
\]

where \( \rho \) is the density (mass per unit volume). If no mass is created or destroyed inside \( V \), this quantity must be equal to the rate of the material flow into the volume \( V \) through its surface \( \Omega \) (Malvern, 1969):

\[
\int_V \frac{\partial \rho}{\partial t} dV = -\int_{\Omega} \rho \cdot \nu \cdot d\Omega \tag{3.2}
\]

where \( \nu \) is the velocity, \( d\Omega \) is a vector with magnitude \( d\Omega \) normal to the surface and counted positive from the inside to the outside. The quantities \( \rho \) and \( \nu \) are all functions of time and of space coordinates. Applying Gauss’s theorem to the surface integral in equation (3.2), we obtain:

\[
\frac{\partial \rho}{\partial t} = -\text{div} \ rho \nu \tag{3.3}
\]

Equation (3.3) is valid for an arbitrary volume \( V \), which expresses the fact that the total mass is conserved, i.e. that the total mass in any volume element of the system can only change if matter flows into (or out of) the volume element. This equation has the form of a so-called balanced equation: the local change of the density is equal to the negative divergence of the flow of mass. The continuity equation in the vector form of equation (3.3) is independent of any choice of coordinates.

The mass equation can also be written in an alternative form by introducing the substantial time derivative (Groot and Mazur, 1962):

\[
\frac{d}{dt} = \frac{\partial}{\partial t} + \nu \cdot \text{grad} \tag{3.4}
\]

With the help of equation (3.4), equation (3.3) becomes (Groot and Mazur, 1962):
\[
\frac{d\rho}{dt} = -\rho \text{div} \mathbf{v}
\]  

(3.5)

With the specific volume \( v = \rho^{-1} \), formula (3.5) may also be written as (Groot and Mazur, 1962):

\[
\rho \frac{dv}{dt} = \text{div} \mathbf{v}
\]

(3.6)

Finally the following relation is valid for an arbitrary local property \( a \) that may be a scalar or a component of a vector or tensor (Groot and Mazur, 1962):

\[
\rho \frac{da}{dt} = \frac{\partial a}{\partial t} + \text{div} a \rho \mathbf{v}
\]

(3.7)

which is a consequence of the equation (3.3) and equation (3.4). We can verify equation (3.7) directly. According to equation (3.4), the left-hand side of equation (3.7) is

\[
\rho \frac{da}{dt} = \rho \frac{\partial a}{\partial t} + \rho \mathbf{v} \cdot \text{grad} a
\]

According to equation (3.3), the right side of equation (3.7) is

\[
\frac{\partial a}{\partial t} + \text{div} a \rho \mathbf{v} = a \frac{\partial \rho}{\partial t} + \rho \frac{\partial a}{\partial t} + a \text{div} \rho \mathbf{v} + \rho \mathbf{v} \cdot \text{grad} a
\]

\[
= a(-\text{div} \rho \mathbf{v}) + \rho \frac{\partial a}{\partial t} + a \text{div} \rho \mathbf{v} + \rho \mathbf{v} \cdot \text{grad} a
\]

\[
= \rho \frac{\partial a}{\partial t} + \rho \mathbf{v} \cdot \text{grad} a
\]

So equation (3.7) is true.

### 3.2.2 Momentum Principle

The momentum principle for a collection of particles states that the time rate of the change in the total momentum for a given set of particles equals to the vector sum of
all the external forces acting on the particles of the set, provided Newton’s Third Law of action and reaction governs the initial forces (Malvern, 1969). Consider a given mass of the medium, instantaneously occupying a volume \( V \) bounded by surface \( \Omega \) and acted upon by external surface \( t \) and body force \( b \). Then the momentum principle can be expressed as (Malvern, 1969):

\[
\int_{\Omega} t d\Omega + \int_{V} \rho b dV = \frac{d}{dt} \int_{V} \rho v dV
\]  

(3.8)

or in rectangular coordinates:

\[
\int_{\Omega} t_i d\Omega + \int_{V} \rho b_i dV = \frac{d}{dt} \int_{V} \rho v_i dV
\]  

(3.9)

Substituting \( t_i = \sigma_{ji} n_j \) and transforming the surface integral by using the divergence theorem, we obtain (Malvern, 1969):

\[
\int_{V} \left( \frac{\partial \sigma_{ji}}{\partial x_j} + \rho b_j - \rho \frac{dv_i}{dt} \right) dV = 0
\]  

(3.10)

for an arbitrary volume \( V \). Whence at each point we have (Malvern, 1969):

\[
\rho \frac{dv_i}{dt} = \frac{\partial \sigma_{ji}}{\partial x_j} + \rho b_i
\]  

(3.11)

where \( n_j \) is the component of the normal unit vector \( n \), \( v_i (i = 1,2,3) \) is a Cartesian component of \( v \), and where \( x_j (j = 1,2,3) \) is the Cartesian coordinates. The quantities \( \sigma_{ji} (i, j = 1,2,3) \) and \( b_i (i = 1,2,3) \) are the Cartesian components of the stress tensor \( \sigma \) and body force \( b \) respectively. For a nonpolar case the stress tensor \( \sigma \) is symmetric, namely,

\[
\sigma_{ij} = \sigma_{ji} \quad (i, j = 1,2,3)
\]  

(3.12)

In tensor notation equation (3.11) are written as (Groot and Mazur, 1962):
\[ \rho \frac{d \mathbf{v}}{dt} = \text{Div} \sigma + \rho \mathbf{b} \quad (3.13) \]

From a microscopic point of view, the stress tensor \( \sigma \) results from the short-range interactions between the particles of the system, whereas \( \mathbf{b} \) contains the external forces as well as a possible contribution from long-range interactions in the system.

Using relation (3.7), the equation of motion (3.13) can also be written as:

\[ \frac{\partial \rho \mathbf{v}}{\partial t} = -\text{Div}(\rho \mathbf{w} \mathbf{v} - \sigma) + \rho \mathbf{b} \quad (3.14) \]

where \( \mathbf{w} = \mathbf{v} \otimes \mathbf{v} \) is an ordered (dyadic) product. This equation also has the form of a balance equation for the momentum density \( \rho \mathbf{v} \). In fact one can interpret the quantity \( (\rho \mathbf{w} \mathbf{v} - \sigma) \) as a momentum flow with a convective part \( \rho \mathbf{w} \mathbf{v} \), and the quantity \( \rho \mathbf{b} \) as a source of momentum.

It is also possible to derive from equation (3.11) a balance equation for the kinetic energy of the center of gravity motion by multiplying both members with the component \( v_i \) of \( \mathbf{v} \) and summing over \( i \)

\[ \rho \frac{d \frac{1}{2} \mathbf{v}^2}{dt} = \sum_{i,j=1}^{3} \frac{\partial}{\partial x_j} (\sigma_{j} v_i) - \sum_{i,j=1}^{3} \sigma_{j} \frac{\partial}{\partial x_j} v_i + \rho b_i v_i \quad (i = 1,2,3) \quad (3.15) \]

or in tensor notation

\[ \rho \frac{d \frac{1}{2} \mathbf{v}^2}{dt} = \text{div}(\sigma \cdot \mathbf{v}) - \sigma : \mathbf{L} + \rho \mathbf{b} \cdot \mathbf{v} \quad (3.16) \]

where \( \mathbf{L} = \text{Grad} \mathbf{v} \) is the spatial gradient of the velocity. \( \mathbf{L} \) can be written as the sum of a symmetric tensor \( \mathbf{D} \) called the rate of deformation tensor or the stretching tensor and a skew symmetric tensor \( \mathbf{W} \) called the spin tensor or the vorticity tensor as follows (Malvern, 1969):
\[ L = D + W \] (3.17)

where \( D = \frac{1}{2} (L + L^T) \), \( W = \frac{1}{2} (L - L^T) \).

Since \( W \) is skew symmetric, while \( \sigma \) is symmetric, it follows that

\[ \sigma : \text{Grad} \psi = \sigma_{ij} L_{ij} = \sigma_{ij} D_{ij} = \sigma : D \] (3.18)

We can also establish the relationship between the strain rate \( d\varepsilon/dt \) and the rate of the deformation tensor \( D \) (Malvern, 1969):

\[ \frac{d\varepsilon}{dt} = F^T \cdot D \cdot F \] (3.19)

where \( F \) is the deformation gradient referred to the undeformed configuration. When the displacement gradient components are small compared to unity, equation (3.19) is reduced to (Malvern, 1969):

\[ \frac{d\varepsilon}{dt} \approx D \] (3.20)

With the help of equation (3.7), equation (3.16) becomes:

\[ \frac{\partial \frac{1}{2} \rho \varepsilon^2}{\partial t} = -\text{div} \left( \frac{1}{2} \rho \varepsilon \cdot \varepsilon - \boldsymbol{\sigma} \cdot \varepsilon \right) - \boldsymbol{\sigma} : D + \rho \mathbf{b} \cdot \varepsilon \] (3.21)

For the conservative body forces which can be derived from a potential \( \psi \) independent of time (Groot and Mazur, 1962):

\[ \mathbf{b} = -\text{grad} \psi, \quad \frac{\partial \psi}{\partial t} = 0 \] (3.22)

We can now establish an equation for the rate of change of the potential energy density \( \rho \psi \). In fact it follows from equation (3.3) and equation (3.22) that:

\[ \frac{\partial \rho \psi}{\partial t} = \psi \frac{\partial \rho}{\partial t} + \rho \frac{\partial \psi}{\partial t} = \psi (-\text{div} \rho \varepsilon) \]
\[ = - \text{div} \rho \psi \mathbf{v} + \rho \mathbf{v} \cdot \text{grad} \psi = - \text{div} \rho \psi \mathbf{v} - \rho \mathbf{b} \cdot \mathbf{v} \quad (3.23) \]

Adding equation (3.22) and equation (3.23) for the rate of change of the kinetic energy \( \frac{1}{2} \rho \mathbf{v}^2 \) and the potential energy \( \rho \psi \):

\[ \frac{\partial \rho \left( \frac{1}{2} \mathbf{v}^2 + \psi \right)}{\partial t} = - \text{div} \{ \rho \left( \frac{1}{2} \mathbf{v}^2 + \psi \right) \mathbf{v} - \mathbf{\sigma} \cdot \mathbf{v} \} - \mathbf{\sigma} : \mathbf{D} \quad (3.24) \]

This equation shows that the sum of kinetic and potential energy is not conserved, since a source term appears at the right-hand side.

### 3.2.3 Conservation of Energy

The first law of thermodynamics relates the work done on the system and the heat transfer into the system to the change in energy of the system. Suppose that the only energy transferred to system is by mechanical work done on the system by surface tractions and body forces, by heat exchange through the boundary, and the heat generated within the system by external agencies (inductive heating, for example). According to the principle of conservation of energy, the total energy content within an arbitrary volume \( V \) in the system can only change if energy flows into (out of) the volume considered through its boundary \( \Omega \), which can be expressed as (Malvern, 1969):

\[ \frac{d}{dt} \int_{V} \rho e dV = \int_{\partial V} \mathbf{J}_e \cdot d\mathbf{S} + \int_{V} \rho r dV \quad (3.25) \]

here \( e \) is the energy per unit mass, \( \mathbf{J}_e \) is the energy flux per unit surface and unit time, and \( r \) is the distributed internal heat source of strength per unit mass. We shall refer to \( e \) as the total specific energy, because it includes all forms of energy in the system.
Similarly we shall call \( \mathbf{J}_e \) the total energy flux. With the help of Gauss’s theorem we obtain the differential or local form of the law of conservation of energy:

\[
\frac{\partial \rho e}{\partial t} = - \text{div} \mathbf{J}_e + \rho r
\]  

(3.26)

In order to relate this equation to the previously obtained equation (3.24) for the kinetic and potential energy, we must specify what are the various contributions to the energy \( e \) and the flux \( \mathbf{J}_e \). The total specific energy \( e \) includes the specific kinetic energy \( \frac{1}{2} \mathbf{v}^2 \), the specific potential energy \( \psi \) and the specific internal energy \( u \) (Groot and Mazur, 1962):

\[
e = \frac{1}{2} \mathbf{v}^2 + \psi + u
\]  

(3.27)

From a macroscopic point of view this relation can be considered as the definition of internal energy, \( u \). From a microscopic point of view, \( u \) represents the energy of thermal agitation as well as the energy due to the short-range molecular interactions. Similarly, the total energy flux includes a convective term \( \rho \mathbf{v} \), an energy flux \( \mathbf{\sigma} \cdot \mathbf{v} \) due to the mechanical work performed on the system, and finally a heat flux \( \mathbf{J}_q \) (Groot and Mazur, 1962):

\[
\mathbf{J}_e = \rho \mathbf{v} - \mathbf{\sigma} \cdot \mathbf{v} + \mathbf{J}_q
\]  

(3.28)

This equation may be also considered as defining the heat flux \( \mathbf{J}_q \). Then the heat flowing rate per unit mass is:

\[
\rho \frac{dq}{dt} = - \text{div} \mathbf{J}_q
\]  

(3.29)
where \( q \) is the heat flowing into the system per unit mass. If we subtract equation (3.24) from equation (3.26), we obtain, using also equation (3.27) and equation (3.28), the balance equation for the internal energy \( u \):

\[
\frac{\partial \rho u}{\partial t} = -\text{div}\{\rho \mathbf{u} + \mathbf{J}_q\} + \mathbf{\sigma} : \mathbf{D} + \rho r \quad (3.30)
\]

It is apparent from equation (3.30) that the internal energy \( u \) is not conserved. In fact a source term appears which is equal but of opposite sign to the source term of the balance equation (3.24) for kinetic and potential energy.

With the help of equation (3.7), equation (3.30) may be written in an alternative form:

\[
\rho \frac{du}{dt} = -\text{div}\mathbf{J}_q + \mathbf{\sigma} : \mathbf{D} + \rho r \quad (3.31)
\]

The total stress tensor \( \mathbf{\sigma} \) can be split into a scalar hydrostatic pressure part \( p \) and a deviatoric stress tensor \( \mathbf{\sigma}' \) (Malvern, 1969):

\[
\mathbf{\sigma} = -p \mathbf{I} + \mathbf{\sigma}' \quad (3.32)
\]

where \( \mathbf{I} \) is the unit matrix with element \( \delta_{ij} \) (if \( i = j \); \( \delta_{ij} = 0 \), if \( i \neq j \)), \( p = -\frac{1}{3} \sigma_{kk} \).

With the help of equation (3.32), equation (3.31) becomes:

\[
\rho \frac{du}{dt} = -\text{div}\mathbf{J}_q - p \text{div}\mathbf{v} + \mathbf{\sigma}': \mathbf{D} + \rho r \quad (3.33)
\]

where use has been made of the equality

\[
\mathbf{I} : \mathbf{D} = \mathbf{I} : \text{Grad} \mathbf{v} = \sum_{i,j=1}^{3} \delta_{ij} \frac{\partial}{\partial x_j} v_i = \sum_{i=1}^{3} \frac{\partial}{\partial x_i} v_i = \text{div} \mathbf{v}
\]

With equation (3.6), the first law of thermodynamics can finally be written in the form:
\[
\frac{du}{dt} = -v \text{div } J_q - p \frac{dv}{dt} + v \sigma : D + r \quad \text{or}
\]
\[
\frac{du}{dt} = -v \text{div } J_q + v \sigma : D + r
\]  
(3.34)

where \( v \equiv \rho^{-1} \) is the specific volume.

### 3.3 Entropy Law and Entropy Balance

Thermodynamics in the traditional sense is concerned with the study of reversible transformation. For an irreversible process in which the thermodynamic state of a solid changes from some initial state to a current state, it can be assumed that such a process can occur along an imaginary reversible isothermal path. The processes defined in this way will be thermodynamically admissible if, at any instant of evolution, the Clausius-Duhem inequality is satisfied.

According to the principles of thermodynamics, two more new variables: temperature \( T \) and entropy \( S \), are introduced for any macroscopic system. The entropy expresses a variation of energy associated with a variation in the temperature (Lemaitre and Chaboche, 1990). The entropy of the universe, taken as a system plus whatever surroundings are involved in producing the change within the system, can only increase. Changes in the real world are always irreversible processes because of friction, which results in the production of entropy and thus a permanent change in the universe (Dehoff, 1993).

The variation of the entropy \( dS \) may be written as the sum of two and only two terms for a closed system (Groot and Mazur, 1962):

\[
dS = dS_e + dS_i
\]  
(3.35)
where $dS_e$ is the entropy derived from the transfer of heat from external sources across the boundary of the system, and $dS_i$ is the entropy produced inside the system. The second law of thermodynamics states that $dS_i$ must be zero for any reversible (or equilibrium) transformation and positive for irreversible transformation of the system, namely (Groot and Mazur, 1962):

$$dS_i \geq 0$$

(3.36)

The entropy supplied, $dS_e$, on the other hand may be positive, zero or negative, depending on the interaction of the system with its surroundings.

As we know, thermodynamics in the traditional sense is concerned with the study of the reversible transformation for which the equality in equation (3.36) holds. For an irreversible process in which the thermodynamic state of a solid changes from some initial state to a current state, it is assumed that such a process can occur along an imaginary reversible isothermal path which consists of a two-step sequence (Krajcinovic, 1996). This is the so-called local equilibrium assumption, which postulates that the thermodynamic state of a material medium at a given point and instant, is completely defined by the knowledge of the values of a certain number of variables at that instant. The method of local state implies that the laws which are valid for the macroscopic system remain valid for infinitesimally small parts of it, which is in agreement with the point of view currently adopted in the macroscopic description of a continuous system. This method also implies, on a microscopic model, that the local macroscopic measurements performed on the system are really measurements of the properties of small parts of the system, which still contain a large number of the constituting particles. This hypothesis of “local equilibrium” can, from a macroscopic point of view, only be
justified by virtue of the validity of the conclusions derived from it. Ultrarapid phenomena for which the time scale of the evolutions are at the same order as the relaxation time for a return to thermodynamic equilibrium are excluded from this theory’s field of application (Lemaitre and Chaboche, 1990). The physical phenomena can be described with a precision which depends on the choice of the nature and the number of state variables. The processes defined in this way will be thermodynamically admissible if, at any instant of evolution, the Clausius-Duhem inequality is satisfied.

In irreversible thermodynamics, one of the important objectives is to relate the \( dS_i \), the internal entropy production, to the various irreversible phenomena which may occur inside the system. Before calculating the entropy production in terms of quantities which characterize the irreversible phenomena, we shall rewrite equation (3.35) and equation (3.36) in a form which is more suitable for the description of the systems in which the densities of the extensive properties (such as mass and energy considered in conservation laws) are continuous functions of spatial coordinates (Groot and Mazur, 1962):

\[
S = \int V \rho_s dV 
\]

\[
\frac{dS_e}{dt} = -\int_{\Omega} J_{S,\text{tot}} \cdot d\Omega \tag{3.38}
\]

\[
\frac{dS_i}{dt} = \int V \gamma dV \tag{3.39}
\]

where \( s \) is the entropy per unit mass, \( J_{S,\text{tot}} \) is the total entropy flux which is a vector that coincides with the direction of entropy flow and has a magnitude equal to the entropy
crossing unit area perpendicular to the direction of flow per unit time, and $\gamma$ is the entropy source strength or entropy production per unit volume and unit time.

With equation (3.37), equation (3.38) and equation (3.39), formula (3.35) may be written, using Gauss’s theorem, in the form (Groot and Mazur, 1962):

$$\int_{V}^{\gamma} \left( \frac{\partial \rho S}{\partial t} + \text{div} \mathbf{J}_{S,\text{tot}} - \gamma \right) dV = 0$$

(3.40)

where the divergence of $\mathbf{J}_{S,\text{tot}}$ simply represents the net entropy leaving unit volume per unit time. From this relation, it follows, since equation (3.40) must be hold for an arbitrary volume $V$, that:

$$\frac{\partial \rho S}{\partial t} = - \text{div} \mathbf{J}_{S,\text{tot}} + \gamma$$

(3.41)

$$\gamma \geq 0$$

(3.42)

These two formulations are the local forms of equation (3.35) and equation (3.36), i.e. the local mathematical expressions for the second law of thermodynamics. Equation (3.41) is formally a balance equation for the entropy density $\rho S$ with a source $\gamma$ which satisfies the important inequality (3.42). With the help of equation (3.7), equation (3.41) can be rewritten in a slightly different form:

$$\rho \frac{ds}{dt} = - \text{div} \mathbf{J}_{s} + \gamma$$

(3.43)

where the entropy flux $\mathbf{J}_{s}$ is the difference between the total entropy flux $\mathbf{J}_{S,\text{tot}}$ and a convective term $\rho \mathbf{v}$:

$$\mathbf{J}_{s} = \mathbf{J}_{S,\text{tot}} - \rho \mathbf{v}$$

(3.44)
For application in continuum mechanics, we must relate the changes in the properties of the system to the rate of change in entropy, which will enable us to obtain more explicit expressions for the entropy flux $J_s$ and the entropy source strength $\gamma$ that appears in equation (3.43).

We postulate the existence of a thermodynamic potential from which the state laws can be derived. Without entering the details, let us say that the specification of a function with a scalar value, concave with respect to $T$, and convex with respect to other variables, allows us to satisfy a priori the conditions of thermodynamic stability imposed by Clausius-Duhem inequality. Here we choose the specific Helmholtz free energy $\varphi$, which is defined as the difference between the specific internal energy density $u$ and the product between the absolute temperature $T$ and specific entropy $s$

$$\varphi = u - Ts$$

(3.45)

Differentiating this and with the help of the law of conservation of energy, we have

$$d\varphi = du - Tds - sdT$$

$$= \delta q + \delta w - Tds - sdT$$

$$= \delta q + (\delta w^d + \delta w^e) - Tds - sdT$$

$$= (\delta q + \delta w^d - Tds) + (\delta w^e - sdT)$$

where $q$ is the total heat flowing into the system per unit mass, including the conduction through the surface and the distributed internal heat source, $w$ is the total work done on the system per unit mass by external pressure and body force, $w^d$ is the lost energy associated with the total work, which is generally dissipated in the form of heat, $w^e$ is the elastic energy associated with the total work. For the quantitative treatment of entropy for irreversible processes, let’s introduce the definition of entropy for irreversible processes:
\[ ds = \frac{\delta q + \delta w^e}{T} \]  
(3.46)

With the help of equation (3.46), we have

\[ Tds = du - dw^e \]  
(3.47)

This is the Gibbs relation which combines the first and second laws. From the definition of the entropy, we also have

\[ dw^e = d\varphi + sdT \]  
(3.48)

The Helmholtz free energy is the isothermal recoverable elastic energy. It should be pointed out that the specific elastic energy \( w^e \), namely the work stored in the system per unit mass during a process, is not a function of the process path. It depends only on the end states of the process for a given environmental temperature. The elastic energy is frequently also referred to as the available energy of the process. The elastic energy is the maximum amount of work that could be produced by a device between any given two states. If the device is work absorbing, the elastic energy work of the process is the minimum amount of work that must be supplied (Li, 1989).

In order to find the explicit form of the entropy balance equation (3.43), we insert the expressions (3.34) for \( du/\Omega \) into equation (3.47) with the time derivatives given by equation (3.4):

\[ \rho \frac{ds}{dt} = -\text{div} \mathbf{J}_q - \frac{1}{T} \sigma : \mathbf{D} + \frac{\rho}{T} \frac{dw^e}{dt} + \frac{\rho r}{T} \]  
(3.49)

Noting that

\[ \frac{\text{div} \mathbf{J}_q}{T} = \text{div} \frac{\mathbf{J}_q}{T} + \frac{1}{T^2} \mathbf{J}_q \cdot \text{grad} T \]

it is easy to cast equation (3.49) into the form of a balance equation (3.43):
From comparison with equation (3.43) it follows that the expressions for the entropy flux and the entropy production rate are given by:

\[ \mathbf{J}_s = \frac{\mathbf{J}_q}{T} \]  

(3.51)

\[ \gamma = \frac{1}{T} \mathbf{D} : \mathbf{\sigma} - \frac{\rho}{T} \frac{dw^e}{dt} - \frac{1}{T^2} \mathbf{J}_q \cdot \text{grad} T + \frac{\rho r}{T} \]  

(3.52)

Equation (3.51) shows that for the closed systems, the entropy flow consists of only one part: the “reduced” heat flow \( \mathbf{J}_q/T \). Equation (3.52) represents the entropy production by the internal dissipations. The sum of the first two terms is called the intrinsic dissipation or mechanical dissipation. It consists of plastic dissipation plus the dissipation associated with the evolution of other internal variables; it is generally dissipated by the volume element in the form of heat. The last two terms are the thermal dissipation due to the conduction of heat and the internal heat source. The structure of the expression for \( \gamma \) is that of a bilinear form: it consists of a sum of products of two factors. One of these factors in each term is a flow quantity (heat flow \( \mathbf{J}_q \), momentum flow or pressure tensor \( \mathbf{\sigma} \) ) already introduced in the conservation of laws. The other factor in each term is related to a gradient of an intensive state variable (gradients of temperature and velocity). These quantities which multiply the fluxes in the expression for the entropy production are called thermodynamic forces.

The way in which the separation of the right-hand side of equation (3.49) into the divergence of a flux and a source term has been achieved may at first sight seem to be to some extent arbitrary. The two parts of equation (3.50) must, however, satisfy a number
of requirements which determine this separation uniquely (Groot and Mazur, 1962). The entropy source strength $\gamma$ must be zero if the thermodynamic equilibrium conditions are satisfied within the system. Another requirement which equation (3.52) must satisfy is that it be invariant under the transformation of different reference frames, since the notions of reversible and irreversible behavior must be invariant under such a transformation. It can be seen that equation (3.52) satisfies these requirements. Finally it may be noted that equation (3.50) also satisfies the Clausius-Duhem inequality:

$$\sigma : D - \rho \left( \frac{d\varphi}{dt} + s \frac{dT}{dt} \right) - J_q \cdot \frac{\nabla T}{T} \geq 0$$  \hspace{1cm} (3.53)$$

Between two particles of a solid body which are at different temperatures, heat is transferred only by conduction, a process which takes place at the molecular and atomic levels. The law of heat conduction for isotropic bodies may be stated as follows (Boley and Weiner, 1988):

$$J_q = -k \nabla T$$  \hspace{1cm} (3.54)$$

where $k$, with typical units of $Btu/ft\cdot hr\cdot ^\circ F$, is termed the thermal conductivity of the solid and where $J_q$ is the heat flux.

This law of heat conduction was stated first by Fourier who based it on experimental observation. Fourier’s law expresses a linear relation between the heat flux vector $J_q$ and its dual variable $\nabla T$. Since solid, opaque bodies are of primary interest here, heat is transferred from point to point within this body solely by conduction. The field equation of the boundary-value problem will, therefore, always be some form of the Fourier heat conduction equation. Of course, heat may be transferred to the surface of the
body by other modes of heat transfer which correspond to various thermal boundary conditions.

Then the expression for the internal entropy source can be simplified as:

$$\gamma = \frac{1}{T} \mathbf{\sigma} : \mathbf{D} - \frac{\rho}{T} \frac{d}{dt} \frac{d}{dt} + \frac{k}{T^2} \text{grad} T^2 + \frac{\rho r}{T}$$

(3.55)

### 3.4 Fully Coupled Thermo-Mechanical Equations

The formalism of continuum mechanics and thermodynamics requires the existence of a certain number of state variables. We limit ourselves to two observable variables: the temperature $T$ and the total strain $\epsilon$, as they are the only ones which occur in elasticity. For dissipative phenomena the current state also depends on the past history that is represented, in the method of local state, by the values at each instant of other variables called internal variables. Plasticity and viscoplasticity require the introduction of the plastic (or viscoplastic) strain $\epsilon^p$ as a variable. Other phenomena, such as hardening, damage and fracture, require the introduction of other internal variables of less obvious nature. These variables represent the internal state of matter (density of dislocations, crystalline of microstructures, configuration of microcracks and cavities, etal.) (Lemaitre and Chaboche, 1990). There is no objective way to choose the nature of the internal variables best suited to the study of a phenomenon. For general study, here these variables will be denoted by $V_k (k = 1, 2, \cdots)$ representing either a scalar or a tensorial variable.

For small strains, the plastic strain is the permanent strain associated with the relaxed configuration which is obtained by elastic unloading, leading to the additive strain decomposition:
\[ \varepsilon = \varepsilon^e + \varepsilon^p \] (3.56)

The relations existing between the energy, stress tensor and strain tensor can be obtained using the formalism of thermodynamics with internal variables. Here we choose the specific Helmholtz free energy \( \varphi \), which depends on observable variables and internal variables:

\[ \varphi = (\varepsilon, T, \varepsilon^e, \varepsilon^p, V_k) \] (3.57)

For small strains, the strains appear only in the form of their additive decomposition, so that

\[ \varphi((\varepsilon - \varepsilon^p), T, V_k) = \varphi(\varepsilon^e, T, V_k) \] (3.58)

which shows that (Lemaitre and Chaboche, 1990):

\[ \frac{\partial \varphi}{\partial \varepsilon^e} = \frac{\partial \varphi}{\partial \varepsilon} = -\frac{\partial \varphi}{\partial \varepsilon^p} \] (3.59)

and the following expressions define the thermodynamic laws (Lemaitre and Chaboche, 1990):

\[ \sigma = \rho \frac{\partial \varphi}{\partial \varepsilon^e} \] (3.60)

\[ s = -\frac{\partial \varphi}{\partial T} \] (3.61)

\[ A_k = \rho \frac{\partial \varphi}{\partial V_k} \] (3.62)

where \( A_k \) is the thermodynamic force associated with the internal variables \( V_k \), \( s \), \( \sigma \) and \( A_k \) constitute the associated variables. The vector formed by the variables is the gradient of the function \( \varphi \) in the space of the variables \( T \), \( \varepsilon^e \) and \( V_k \). This vector is normal to the surface \( \varphi = \text{constant} \).
Let us return to the equation of the conservation of energy for small strains (from equation (3.20) and equation (3.31)):

$$\rho \dot{\mathbf{u}} = - \text{div} \mathbf{J}_q + \mathbf{\sigma} : \dot{\mathbf{\epsilon}} + \rho r$$

(3.63)

and replace $\rho \dot{\mathbf{u}}$ by the expression derived from equation (3.45):

$$\rho \dot{\mathbf{u}} = \rho \dot{\phi} + \rho s \dot{T} + \rho s \dot{T}$$

(3.64)

and $\dot{\phi}$ and $\dot{s}$ by its expression as a function of the state variables with the help of equation (3.60), equation (3.61) and equation (3.62):

$$\dot{\phi} = \frac{\partial \phi}{\partial \mathbf{\epsilon}^e} \dot{\mathbf{\epsilon}^e} + \frac{\partial \phi}{\partial T} \hat{T} + \frac{\partial \phi}{\partial V_k} \dot{V}_k = \frac{1}{\rho} \mathbf{\sigma} : \dot{\mathbf{\epsilon}^e} - \dot{s} \hat{T} + A_k \dot{V}_k$$

(3.65)

$$\dot{s} = - \frac{\partial^2 \phi}{\partial \mathbf{\epsilon}^e \partial T} \dot{\mathbf{\epsilon}^e} - \frac{\partial^2 \phi}{\partial T^2} \hat{T} - \frac{\partial^2 \phi}{\partial V_k \partial T} \dot{V}_k = - \frac{1}{\rho} \frac{\partial \mathbf{\sigma}}{\partial T} : \dot{\mathbf{\epsilon}^e} + \frac{\partial s}{\partial T} \hat{T} - \frac{1}{\rho} \frac{\partial A_k}{\partial T} \dot{V}_k$$

(3.66)

We obtain:

$$- \text{div} \mathbf{J}_q = \rho T \frac{\partial s}{\partial T} \hat{T} - \mathbf{\sigma} : (\dot{\mathbf{\epsilon}^e} - \dot{\mathbf{\epsilon}^e}) + A_k V_k - \rho r - T \left( \frac{\partial \mathbf{\sigma}}{\partial T} : \dot{\mathbf{\epsilon}^e} + \frac{\partial A_k}{\partial T} \dot{V}_k \right)$$

(3.67)

By introducing the specific heat defined by:

$$C = T \frac{\partial s}{\partial T}$$

(3.68)

and taking into account Fourier’s Law for isotropic materials:

$$\text{div} \mathbf{J}_q = -k \text{div} (\text{grad} T) = -k \nabla^2 T$$

(3.69)

where $\nabla^2$ denotes the Laplacian operator.

We obtain, using $\dot{\mathbf{\epsilon}^p} = \dot{\mathbf{\epsilon}} - \dot{\mathbf{\epsilon}^e}$:

$$k \nabla^2 T = \rho C \hat{T} - \mathbf{\sigma} : \dot{\mathbf{\epsilon}^p} + A_k V_k - \rho r - T \left( \frac{\partial \mathbf{\sigma}}{\partial T} : \dot{\mathbf{\epsilon}^e} + \frac{\partial A_k}{\partial T} \dot{V}_k \right)$$

(3.70)
This is the fully coupled thermo-mechanical equation, which can simulate the evolution of temperature influenced by the mechanical work with properly imposed boundary conditions. \( A_k \dot{V}_k \) represents the nonrecoverable energy stored in the materials corresponding to other dissipated phenomena such as hardening, damage and fracture. It represents only 5-10% of the term \( \sigma : \dot{e}^\nu \) and is often negligible (Lemaitre, J. and Chaboche, J. L. 1990):

\[
A_k \dot{V}_k \approx 0 \quad (3.71)
\]

which results in the fully coupled elastoplastic thermo-mechanical equation:

\[
k \nabla^2 T = \rho C \dot{T} - \sigma : \dot{e}^p - \rho f - T \frac{\partial \sigma}{\partial T} : \dot{e}^e \quad (3.72)
\]

which has been used to simulate the thermal effects on the material behavior by many researchers (Sluzalec et al. 1998, Hong 1999). Equation (3.72) also allows us to calculate heat flux \( J_q \) generated due to elastic and/or inelastic work in a solid body.

For the isotropic linear thermoelastic materials, the stress-strain relationship is:

\[
\sigma_{ij} = \lambda \delta_{ij} \varepsilon_{kk} + 2 \mu \varepsilon_{ij} - (3 \lambda + 2 \mu) \delta_{ij} \alpha (T - T_0) \quad (3.73)
\]

where \( T_0 \) is the reference temperature, \( \alpha \) is the isotropic thermal expansion coefficient, \( \lambda \) and \( \mu \) are the Lame’s coefficients:

\[
\lambda = \frac{v E}{(1 + v)(1 - 2v)}; \quad \mu = \frac{E}{2(1 + v)} \quad (3.74)
\]

If the internal generation of heat created by external sources is neglected, equation (3.70) becomes for isotropic linear thermoelastic materials:

\[
k \nabla^2 T = \rho C \dot{T} + (3 \lambda + 2 \mu) \alpha T \dot{e}_{kk} \quad (3.75)
\]

The last term represents the interconvertibility of the thermal and mechanical energy.
3.5 Damage Evolution Function

Changes are always irreversible processes because of friction, which results in the production of entropy and thus a permanent change in the universe (Dehoff, 1993). Damage is the progressive deterioration which occurs in materials prior to failure. Cumulative damage analysis plays a key role in the life prediction of components and structures subjected to load histories. As a result, many damage models have been proposed in the literature, such as linear damage models, nonlinear damage models, linear elastic fracture mechanics models, continuum damage mechanics models and energy based damage models (Bazant 1991; Bonora et al. 1998; Chaboche, 1988; Chow & Chen 1992; Ju 1989, 1990; Kachanov 1958, 1986; Krajcinovic 1989; Lemaitre 1996; Murakami et al. 1988, 1997; Rabotnov 1969; Shi et al. 1997; Voyiadjis et al. 1996). Damage evolution function based on thermodynamics and statistical mechanics was first introduced by Basaran and Yan (1998), who established a relationship between entropy and damage for solids undergoing plastic deformations. Yet their model is not general enough to account for elastic deformations and to relate entropy production with material stiffness degradation. Basaran and Nie (2004) developed a generalized version of this damage evolution model.

There are many metrics to measure degradation in materials, such as direct measurements of the total crack areas lying on a surface, degradation of the elastic modulus, degradation of ultrasonic wave propagation speed, degradation of the microhardness, change in density, increase in electrical resistance, variation in the cyclic plastic response, change in creep properties, change in acoustic emission properties, remaining life and cumulative hysteresis dissipation. The damage process corresponding
to the degradation of microstructure is, in general, irreversible. During the cumulative damage process, the internal entropy production, which is a measure of disorder in the system, must increase according to the second law of thermodynamics, so that internal entropy production can be used as a criterion for quantification of damage. Entropy in statistical physics and in the thermodynamic sense is really the same thing (Malvern, 1969). The statistical physics interpretation in terms of probability and tendency toward disordered microstates furnishes a physical significance for the otherwise rather abstract thermodynamic concept of entropy. Boltzmann (1898) first used statistical mechanics to give a precise meaning to disorder and established a connection between disorder and entropy for the whole system.

\[ S = k_o \ln W \]  
(3.76)

where \( k_o \) is Boltzmann constant and \( W \) is the disorder parameter which is the probability that the system will exist in the state relative to all the possible states it could be in. Statistical mechanics assigns an exact meaning to the probability of a state and supplies a general expression for \( W \) that employs the idea of the distribution function of a system. This function measures the probability for the coordinates and velocities of the molecules of the system to have specified values at a given time. The relation between the entropy per unit mass and the disorder parameter is given by Basaran and Yan (1998):

\[ s = \frac{R}{m_s} \ln W \]  
(3.77)

where \( s \) is the entropy per unit mass, \( m_s \) is the specific mass, \( R \) is the gas constant.

According to equation (3.77) we have the disorder function as follows:

\[ W = e^{\frac{sm}{R}} \]  
(3.78)
Select an initial reference state of the continuous medium with disorder $W_0$, then the change in disorder at any arbitrary time with respect to the initial reference state is given by:

$$\Delta W = W - W_0 = e^{s_m} - e^{s_{m_0}}$$  \hspace{1cm} (3.79)

where $s_0$ is the entropy for the initial reference state. According to Basaran and Nie (2004), the isotropic damage variable $D$ is defined as the ratio of the change in disorder parameter to the current state disorder parameter with a proportional critical disorder coefficient $D_{cr}$:

$$D = D_{cr} \frac{\Delta W}{W}$$  \hspace{1cm} (3.80)

where $D_{cr}$ allows us to correlate the value of entropy production based damage $D$ with other material coordinates, such as degradation of material stiffness. $D_{cr}$ is easy to determine from experimental data, but it can vary for different loading profiles such as monotonic and cyclic loading.

With the help of equation (3.78) and equation (3.79), the relation between the damage parameter $D$ and the change in entropy can be written as:

$$D = D_{cr} \left[ 1 - e^{\frac{m}{R}(s-s_0)} \right]$$  \hspace{1cm} (3.81)

With the help of equation (3.49) and equation (3.70), the rate of total specific entropy change under the condition of small strains is given by:

$$\frac{ds}{dt} = c \frac{\partial T}{\partial t} - \frac{1}{\rho} \left( \frac{\partial \sigma}{\partial t} : \epsilon^e + \frac{\partial A_k}{\partial t} : V_k \right)$$  \hspace{1cm} (3.82)
where the identity $\mathbf{\sigma} : \mathbf{\dot{\varepsilon}} - \rho \dot{\mathbf{w}}^c = \mathbf{\sigma} : \mathbf{\dot{\varepsilon}}^p - A_k \dot{V}_k$ is used, which represents the total mechanical dissipation rate. Equation (3.82) can also be obtained by its expression as a function of the state variables as same as the equation (3.66).

With the help of equation (3.55), the specific entropy production rate for small strains becomes:

$$\frac{ds}{dt} = \frac{\gamma}{\rho} \frac{\mathbf{\sigma} : \mathbf{\dot{\varepsilon}}^p}{T \rho} + \frac{k}{T^2 \rho} \left| \text{grad} T \right|^2 + \frac{r}{T}$$

(3.83)

where the identity $\mathbf{\sigma} : \mathbf{\dot{\varepsilon}} - \rho \dot{\mathbf{w}}^c = \mathbf{\sigma} : \mathbf{\dot{\varepsilon}}^p - A_k \dot{V}_k$ is also used and $A_k \dot{V}_k$ is omitted.

The fundamental equations governing the temperature, stresses, deformation and the entropy production rate in a continuum medium have been derived in the previous section. From a strict viewpoint these quantities were all interrelated and had to be determined simultaneously. However, for most practical problems the effect of the stresses and deformations upon the temperature distribution is quite small and can be neglected. This procedure allows the determination of the temperature distribution in the solid resulting from prescribed thermal conditions to become the first and independent step of a thermal-stress analysis; the second step of such an analysis is then the determination of the stresses, deformations and damage in the body due to this temperature distribution (Boley and Weiner, 1988). Because the entropy change caused by the heat transfer between systems and surroundings has no influence on the degradation of the materials, only the entropy source strength, namely the entropy created in the system, should be used as a basis for the systematic description of the irreversible processes. So the damage evolution equation (3.73) can be implemented in a numerical analysis procedure, where
\[ \Delta s = \Delta s_j = \int_{t_0}^{t} \frac{\mathbf{\sigma} : \dot{\mathbf{e}}^P}{T^2 \rho} dt + \int_{t_0}^{t} \left( \frac{k}{T^2 \rho} |\text{grad} T|^2 \right) dt + \int_{t_0}^{t} \frac{r}{T} dt \] (3.84)

According to equation (3.84), it is obvious that \( D \geq 0 \) is always satisfied because of the nonnegative entropy source strength. \( D = 0 \) when \( \Delta s = 0 \) and \( D = D_{cr} \) when \( \Delta s \rightarrow \infty \). Equation (3.84) shows that the damage is not only a function of the loading or straining process, but also of the temperature. However, a uniform increase in temperature in a stress free field does not cause any damage.

An irreversible thermodynamic model has been proposed for damage mechanics of inelastic materials. The advantage of the proposed procedure is quite obvious. Instead of separate formulations of constitutive and damage evolution equations in the continuum damage mechanics (CDM) theory, a unified description of CDM is possible only by establishing the constitutive relationship. So the whole problem of modeling the damage phenomenon lies in the determination of the analytical expressions for the constitutive relationship, and its identification in characteristic experiments. The specific functional form of the constitutive relationship depends on the damage mechanism and the deformation itself. Moreover, this unified approach nullifies the need for a damage potential surface.

### 3.6 Damage Coupled Viscoplasticity

The damage coupled material constitutive model is ideally suited to characterize the mutual interaction between the macro-level mechanical properties and material damage due to microstructure degradation. The damage variable can be directly used as the fatigue damage criterion for the numerical model, from which the number of cycles to
failure can be determined. Furthermore, the damage distribution and progressive damage evolution can be obtained.

3.6.1 Effective Stress and Strain Equivalence Principle

Lemaitre (1990) considered a certain section of the representative volume element (RVE) under uniaxial force $F$ as shown in figure 3.1, where $\delta S$ is the initial area of the undamaged section, $\delta S_D$ denotes the lost area as result of damage. $\delta S - \delta S_D$ can be interpreted as the actual area of the section. The values $\delta S$ and $\delta S_D$ are to be understood in the sense of appropriate averaging.

![Figure 3.1 Schematic illustration of definition of damage](image)

The nominal stress can be defined as:

$$\sigma = \frac{F}{\delta S} \quad (3.85)$$

Rabotnov (1969) introduced the concept of effective stress $\tilde{\sigma}$, which relates to the surface that effectively resists the load, namely $(\delta S - \delta S_D)$,

$$\tilde{\sigma} = \frac{F}{\delta S - \delta S_D} \quad (3.86)$$
Kachanov (1986) gave the definition of damage at microscale as the creation of microsurface discontinuities: breaking of atomic bonds and plastic enlargement of microcavities. This isotropic damage variable is defined as

\[ D = \frac{\delta S_D}{\delta S} \]  

(3.87)

So, we have

\[ \tilde{\sigma} = \frac{\sigma}{1 - D} \]  

(3.88)

Lemaitre (1990) assumed that the strain response of the body is modified by damage only through the actual stress. Thus, the stress-strain behavior of the damaged material can be represented by the constitutive equation of the virgin material (without damage) with the stress in it replaced by the effective stress. And this is the strain equivalence principle: “Any strain constitutive equation for a damaged material may be derived in the same way as for a virgin material except that the usual stress is replaced by the effective stress”.

The strain equivalent principle demonstrates the major role of the concept of actual stress. According to the strain equivalence principle, the elastic strain of a damaged material is:

\[ \varepsilon^e = \frac{\tilde{\sigma}}{\tilde{E}} = \frac{1}{E} \frac{\sigma}{1 - D} \]  

(3.89)

So, the Hook's law here has its usual form with the Young's modulus \( E \) being replaced by \( \tilde{E} \). Where \( \tilde{E} \) is the Young’s modulus associated with the damaged status.

In the case of an elastic-plastic deformation when the damage is a result of a large strain, it is natural to assume that damage does not depend on the elastic strain, hence
\[
\frac{dD}{d\varepsilon'} = 0 \quad (3.90)
\]

This condition leads to the relation

\[
D = 1 - \frac{\bar{E}}{E} \quad (3.91)
\]

Hence, the damage may be estimated by measuring the elastic response. Note \(\bar{E}\) can be identified with the unloading modulus. So the change in modulus with strain was considered by the damage parameter \(D\), which reflects the decrease in load carrying ability of particles in particulate composites as they crack or debond.

### 3.6.2 Damage Coupled Isotropic Viscoplasticity

In order to simulate damage behavior of solid materials, there is a need for a progressive constitutive degradation model. Damage mechanics provides basic framework to develop damage evolution models at small strains.

#### 3.6.2.1 Damage Coupled Constitutive Equations

In accordance with the strain equivalence principle and Hook’s law, the elasticity constitutive relationship may be written as:

\[
d\sigma = (1 - D)C^e d\varepsilon' \quad (3.92)
\]

where \(d\varepsilon'\) is the elastic strain increment vector; \(C^e\) is the elastic constitutive matrix, \(d\sigma\) is the total stress increment vector, and \(D\) is the isotropic damage parameter.

Assuming deformations of small strain, the total strain increment can be separated into three components,

\[
\{d\varepsilon\} = \{d\varepsilon^h\} + \{d\varepsilon^c\} + \{d\varepsilon^p\} \quad (3.93)
\]
where $d\varepsilon^\text{th}$, $d\varepsilon^e$ and $d\varepsilon^\text{vp}$ are the incremental thermal, elastic and viscoplastic strains, respectively.

The thermal strain increment is

$$
d\varepsilon^\text{th} = \alpha_T dT \mathbf{I}
$$

where $\alpha_T$ is the coefficient of thermal expansion, $dT$ is the temperature increment, and $\mathbf{I}$ is the second order unit tensor. $\{d\varepsilon^\text{vp}\}$ is viscoplastic strain increment, which can be determined using the viscoplasticity theory.

So the total stress increment can be obtained by:

$$
d\sigma = (1-D) \mathbf{C}^e (d\varepsilon - d\varepsilon^\text{vp} - d\varepsilon^\text{th})
$$

### 3.6.2.2 Damage Coupled Yield Surface

Von-Mises type yield surface with isotropic and kinematic hardening is used in the constitutive model here. Von Mises criterion states that the viscoplastic strain is governed by the elastic shear (or deviatoric) energy density, the so-called $J_2$ theory.

$$
F = q - \bar{\sigma}
$$

where the Mises equivalent stress $q$ is

$$
q = \sqrt{\frac{3}{2}} (\mathbf{S} - \mathbf{a}) : (\mathbf{S} - \mathbf{a})
$$

$\mathbf{S}$ is the deviatoric stress tensor defined by:

$$
\mathbf{S} = \sigma - \frac{1}{3} \sigma_{kk} \mathbf{I}
$$

$\mathbf{a}$ is the deviatoric stress component of back stress tensor corresponding to kinematic hardening.
\( \bar{\sigma} \) is the equivalent yield stress:

\[
\bar{\sigma} = R + \sigma_y
\]  

(3.99)

\( R \) is the evolution of the size of the yield surface corresponding to isotropic hardening; 
\( \sigma_y \) is the initial size of the yield surface. Figure 3.2 shows the yield surface in the principal stress space.

![Figure 3.2 Yield locus in the principal stress space (Lemaitre, et al., 1990)](image)

The kinematic hardening represents an approximation of accounting for the Bauschinger effect. The corresponding deviatoric back stress represents the translation of the center of the yield surface in the deviatoric space. Isotropic hardening stress \( R \) measures the increase in radius of the yield cylinder in the stress space.

Damage has significant effects on the yield surface. In order to model the behavior of a damaged material, the strain equivalence principle is needed. According to the strain equivalence principle, the normal stress is replaced by the effective stress in the
yield function, and all other variables remain unchanged. So the yield function has the same form with the modified Mises equivalent stress:

\[ q^* = \sqrt{\frac{3}{2}} \left[ \frac{S}{1-D} - a \right] \cdot \left( \frac{S}{1-D} - a \right) \]  \hspace{1cm} (3.100)

If the nominal stress \( \sigma \) is used, instead of the effective stress \( \bar{\sigma} \), the yield surface can be written as:

\[ F = q^d - \bar{\sigma}^d \]  \hspace{1cm} (3.101)

with the damage coupled back stress, Mises equivalent stress and yield stress as follows:

\[ a^d = (1 - D) \alpha \]  \hspace{1cm} (3.102)

\[ \bar{\sigma}^d = (1 - D) \bar{\alpha} \]  \hspace{1cm} (3.103)

\[ q^d = \sqrt{\frac{3}{2}} (S - \alpha^d) \cdot (S - \alpha^d) \]  \hspace{1cm} (3.104)

It shows that the damage equally decreases the yield stress, the isotropic strain hardening stress and the back stress.

It is emphasized that the fully coupled elastoplastic thermo-mechanical equation (3.70), the damage evolution function (3.81), the entropy production equation (3.84) and the constitutive equation (3.95) completely characterize the progressive damage behavior of any material.

3.7 Examples

Damage coupled plasticity is ideal for the damage coupled plasticity calculations, either as a rate dependent or as a rate independent model. Damage coupled linear kinematic hardening plasticity and damage coupled isotropic hardening plasticity have
particularly simple forms. Because of this simplicity, the algebraic equations associated with integrating this model are easily developed in terms of a single variable, and the material stiffness matrix can be written explicitly. For simplicity of notation, all quantities not explicitly associated with a time point are assumed to be evaluated at the end of the increment.

### 3.7.1 Damage Coupled Plasticity with Isotropic Hardening

The Mises yield function with associated flow means that there is no volumetric plastic strain, and since the elastic bulk modulus is quite large, the volume change will be small, so that we can define the volume strain as

\[ \varepsilon_{\text{vol}} = I : \varepsilon = \text{trace}(\varepsilon) \]  

(3.105)

where \( I \) is the second order unit tensor.

The deviatoric strain is

\[ \varepsilon = \varepsilon - \frac{1}{3} \varepsilon_{\text{vol}} I = \varepsilon - \frac{1}{3} \Pi : \varepsilon = \left( \Pi - \frac{1}{3} I \otimes I \right) : \varepsilon \]  

(3.106)

where \( \Pi \) is the fourth-order unit tensor.

The equivalent pressure stress

\[ p = -\frac{1}{3} \text{trace}(\sigma) = -\frac{1}{3} I : \sigma \]  

(3.107)

The deviatoric stress is defined as

\[ S = \sigma + pI \]  

(3.108)

The Mises equivalent stress

\[ q = \sqrt{2}(S : S) \]  

(3.109)

where
\[ \frac{3}{2} (\mathbf{S} : \mathbf{S}) = \frac{1}{2} \left[ (\sigma_{11} - \sigma_{22})^2 + (\sigma_{22} - \sigma_{33})^2 + (\sigma_{33} - \sigma_{11})^2 + 6(\sigma_{12}^2 + \sigma_{23}^2 + \sigma_{13}^2) \right] \quad (3.110) \]

Strain rate decomposition is
\[ d\varepsilon = d\varepsilon^{el} + d\varepsilon^{pl} \quad (3.111) \]

Using the standard definition of corotational measures, this can be written in the integrated form as
\[ \varepsilon = \varepsilon^{el} + \varepsilon^{pl} \quad (3.112) \]

The elasticity is linear and isotropic, and may therefore be written in terms of two temperature dependent material parameters bulk modulus \( K \) and shear modulus \( G \), which are readily computed from Young’s modulus \( E \) and Poisson ratio \( \nu \) as
\[ K = \frac{E}{3(1-2\nu)} \quad (3.113) \]
and
\[ G = \frac{E}{2(1+\nu)} \quad (3.114) \]

The elasticity coupled with isotropic damage may then be written in volumetric and deviatoric components as follows:
\[ p = -(1-D)K\varepsilon_{vol} = -(1-D)K I : \varepsilon \quad (3.115) \]
\[ \mathbf{S} = 2(1-D)G\varepsilon^{el} \quad (3.116) \]

The flow rule is:
\[ d\varepsilon^{pl} = d\varepsilon^{pl} n \quad (3.117) \]

where
\[ n = \frac{3}{2} \frac{\mathbf{S}}{q} \quad (3.118) \]
$d\dot{\varepsilon}^{pl}$ is the scalar equivalent plastic strain rate. The evolution of the equivalent plastic strain is obtained from the following equivalent plastic work expression:

$$\sigma_y \dot{\varepsilon}^{pl} = \sigma : \dot{\varepsilon}^{pl} \quad (3.119)$$

which yields

$$\dot{\varepsilon}^{pl} = \sqrt{\frac{2}{3} \dot{\varepsilon}^{pl} : \dot{\varepsilon}^{pl}} \quad (3.120)$$

for isotropic Mises plasticity. Using equation (3.117) and equation (3.118) we can prove this result as follows.

$$\sigma_y \dot{\varepsilon}^{pl} = \sigma : \dot{\varepsilon}^{pl} = (S - pI) : \dot{\varepsilon}^{pl} = S : \dot{\varepsilon}^{pl}$$

Then,

$$\dot{\varepsilon}^{pl} = \frac{S}{\sigma_y} : \dot{\varepsilon}^{pl} = \frac{2}{3} \mathbf{n} : \dot{\varepsilon}^{pl} = \frac{2}{3} \dot{\varepsilon}^{pl} : \dot{\varepsilon}^{pl} = \frac{2}{3} \dot{\varepsilon}^{pl} : \dot{\varepsilon}^{pl}$$

Therefore, we have

$$\dot{\varepsilon}^{pl} = \sqrt{\frac{2}{3} \dot{\varepsilon}^{pl} : \dot{\varepsilon}^{pl}}$$

The plasticity requires that the material satisfy a uniaxial-stress, plastic-strain, and strain-rate relationship. If the material is rate independent this is the yield condition:

$$q = (1-D)\sigma^0 \left( \varepsilon^{pl}, T \right) \quad (3.121)$$

If the material is rate dependent, the relationship is the uniaxial flow rate definition:

$$\dot{\varepsilon}^{pl} = h \left( \frac{q}{1-D}, \varepsilon^{pl}, T \right) \quad (3.122)$$

where $h$ is a known function.

Integrating this relationship by the backward Euler method gives
\[ \Delta \bar{e}^{pl} = h\left(\frac{q}{1-D},\bar{e}^{pl},T\right) \Delta t \]  

(3.123)

The backward Euler method is an unconditional stable and second-order accurate algorithm. This equation can be inverted (numerically, if necessary) to give \( q \) as a function of \( \bar{e}^{pl} \) at the end of the increment. Thus both the rate independent model and the integrated rate dependent model give the general uniaxial form:

\[ q = (1-D)\bar{\sigma}\left(\bar{e}^{pl},T\right) \]  

(3.124)

where \( \bar{\sigma} = \sigma^0 \) for the rate independent model, and \( \bar{\sigma} \) is obtained by the inversion of equation (3.123) for the rate dependent model.

In any increment when plastic flow is occurring (which is determined by evaluating \( q \) based on purely elastic response and finding that its value exceeds \((1-D)\bar{\sigma})\), these equations must be integrated and solved for the state at the end of the increment. The integration is done by applying the backward Euler method to the flow rule (equation (3.117)), giving

\[ \Delta e^{pl} = \Delta \bar{e}^{pl} \mathbf{n} \]  

(3.125)

Combining this with the deviatoric elasticity (equation (3.116)) and the integrated strain rate decomposition (equation (3.112)) gives

\[ S = 2(1-D)G\left(e^{pl},\Delta e, \Delta \bar{e}^{pl} \mathbf{n}\right) \]  

(3.126)

Then using the integrated flow rule (equation (3.125)), together with the Mises definition of the flow direction \( \mathbf{n} \), this becomes,

\[ \left(1+3(1-D)\frac{G}{q}\Delta \bar{e}^{pl}\right)S = S^{\nu} \]  

(3.127)

where
\[ S^p = 2(1 - D)G\hat{e} \]  
(3.128)

\[ \hat{e} = e^p\big|_{t} + \Delta e \]  
(3.129)

With the help of equation (3.109), taking the inner product of equation (3.127) with itself gives

\[ q + 3(1 - D)G\Delta\bar{\varepsilon}^p = q^p \]  
(3.130)

where

\[ q^p = \sqrt{\frac{2}{3} (S^p : S^p)} \]  
(3.131)

where \( q^p \) is the elastic predictor based on purely elastic behavior:

The Mises equivalent stress \( q \) must satisfy the uniaxial form defined in equation (3.124), so that, from equation (3.130),

\[ q^p - 3(1 - D)G\Delta\bar{\varepsilon}^p - (1 - D)\bar{\sigma} = 0 \]  
(3.132)

This is a nonlinear equation for \( \Delta\bar{\varepsilon}^p \) in the general case, which can be solved iteratively by Newton’s method (\( x_{n+1} = x_n + f(x_n)/f'(x_n) \)):

\[ c^p\big|_k = \frac{q^p - 3(1 - D)G\Delta\bar{\varepsilon}^p\big|_k - (1 - D)\bar{\sigma}\big|_k}{(1 + D)(3G + H)} \]  
(3.133)

\[ \Delta\bar{\varepsilon}^p\big|_{k+1} = \Delta\bar{\varepsilon}^p\big|_k + c^p\big|_k \]  
(3.134)

where

\[ H = (1 - D)\frac{\partial\bar{\sigma}}{\partial\bar{\varepsilon}^p}\big|_k \]  
(3.135)

and we iterate until convergence is achieved. Once \( \Delta\bar{\varepsilon}^p \) is known, the solution is fully defined.

Using equation (3.124):
\[ q = (1 - D) \bar{\sigma}(\bar{e}^{pl}, T) \]  

(3.136)

Using equation (3.127) and equation (3.130):
\[
S^{pr} = \frac{S^{pr}}{1 + 3(1 - D)q \Delta \bar{e}^{pl}} = \frac{q}{q^{pr}} S^{pr}  
\]  

(3.137)

Using equation (3.118):
\[ n = \frac{3}{2} \frac{S}{q} \]  

(3.138)

Using equation (3.125):
\[ \Delta e^{pl} = \Delta \bar{e}^{pl} n \]  

(3.139)

For cases where three direct strain components are provided by the kinematic solution, equation (3.115) defines:
\[ p = -(1 - D)K \epsilon_{vol} = -\frac{1}{3} \sigma^{pr}_{kk} \]  

(3.140)

So that the solution is then fully defined, and the material stiffness matrix can be derived without the need for matrix inversion as follows. Taking the variation of equation (3.137) with respect to all quantities at the end of the increment gives:
\[ \partial S = q \partial \left( \frac{S^{pr}}{q^{pr}} \right) + \frac{S}{q} \partial q \]  

(3.141)

From equation (3.128),
\[ \partial S^{pr} = 2(1 - D)G \partial \epsilon \]  

(3.142)

And from equation (3.131),
\[ \partial q^{pr} = 3(1 - D)G \frac{S^{pr}}{q^{pr}} : \partial \epsilon = \frac{3(1 - D)G}{q} S : \partial \epsilon \]  

(3.143)

where equation (3.137) and equation (3.142) have been used.
So,

\[
\frac{\partial}{\partial q} \left( \frac{S}{q} \right) = \frac{\partial}{\partial q} S = \frac{2(1-D)G}{q} \partial \hat{e} - \frac{3(1-D)G}{q^2 q'} S \otimes S : \partial \hat{e} \]

(3.144)

where equation (3.137) and equation (3.143) have been used.

From equation (3.124),

\[
\hat{e} = (1-D)H \hat{e} \]

(3.145)

and from equation (3.130),

\[
\hat{e} + 3(1-D)G \hat{e} = \hat{e} \]

(3.146)

Combining equation (3.145), equation (3.146) and equation (3.143):

\[
\hat{e} = \frac{3G}{(3G + H)q} S : \partial \hat{e} \]

(3.147)

So,

\[
\hat{e} = \frac{3(1-D)G}{(3G + H)q} S : \partial \hat{e} \]

(3.148)

Combining these results with equation (3.141) gives:

\[
\hat{e} = 2(1-D)G \frac{q}{q'} \partial \hat{e} - \frac{3(1-D)G}{q^2} \left[ \frac{q}{q'} - \frac{H}{3G + H} \right] S \otimes S : \partial \hat{e} \]

(3.149)

So we have

\[
\hat{e} = \left[ Q \mathbf{1} - R S \otimes S \right] : \partial \hat{e} \]

(3.150)

where

\[
Q = 2(1-D)G \frac{q}{q'} \]

(3.151)

\[
R = \frac{3(1-D)G}{q^2} \left[ \frac{q}{q'} - \frac{H}{3G + H} \right] = \frac{9(1-D)G^2 (q - (1-D)H \Delta \hat{e})}{q^2 q' (3G + H)} \]

(3.152)
For all cases where three direct strains are defined by the kinematic solution the material stiffness is completed by (from equation (3.115))

$$\ddot{\sigma} = -(1 - D)K\mathbf{I} : \ddot{\varepsilon}$$

(3.153)

so that, since (from equation (3.108))

$$\sigma = S - p\mathbf{I}$$

(3.154)

and (from equation (3.106))

$$\ddot{\varepsilon} = \dot{\varepsilon} = (\mathbf{I} - \frac{1}{2} \mathbf{I} \otimes \mathbf{I}) : \ddot{\varepsilon}$$

(3.155)

Because

$$\mathbf{e} = \dot{\mathbf{e}} + \mathbf{e}^p$$

(3.156)

We have

$$\ddot{\sigma} = \left[\left((1 - D)K - \frac{1}{2} Q\right) \otimes \mathbf{I} + Q\mathbf{I} - R\mathbf{S} \otimes S\right] \ddot{\varepsilon}$$

(3.157)

Equation (3.157) can also be written in an alternate form:

$$\Delta \sigma_{ij} = \lambda^* \Delta \varepsilon_{ij} + 2\mu^* \Delta \varepsilon_{ij} + \left(\frac{1 - D}{1 + H/3G} - 3\mu^* \right) \eta_{ij} \eta_{kl} \Delta \varepsilon_{kl}$$

(3.158)

where

$$\mu^* = (1 - D)Gq/q^p$$

(3.159)

$$\lambda^* = (1 - D)K - \frac{2}{3} \mu^*$$

(3.160)

$$\eta_{ij} = S_{ij}^p / q^p$$

(3.161)

Using equation (3.137), equation (3.140) and equation (3.154), we have

$$\sigma_{ij} = \eta_{ij} q + \frac{1}{3} \delta_{ij} \sigma_{kk}^p$$

(3.162)
3.7.2 Damage Coupled Plasticity with Linear Kinematic Hardening

The Mises equivalent stress is defined as

\[
q = \sqrt{\frac{3}{2} (\mathbf{S} - \mathbf{a}) : (\mathbf{S} - \mathbf{a})}
\]  

(3.163)

where \( \mathbf{a} \) is the backstress, which gives the center of the yield surface in deviatoric stress space.

The flow rule is

\[
d \mathbf{e}^{pl} = d \bar{\varepsilon}^{pl} \mathbf{n}
\]  

(3.164)

where

\[
\mathbf{n} = \frac{3}{2} \frac{[\mathbf{S} - \mathbf{a}]}{q}
\]  

(3.165)

and \( d \bar{\varepsilon}^{pl} \) is the scalar equivalent plastic strain rate.

Prager-Ziegler (linear) kinematic hardening model is:

\[
d \mathbf{a} = \frac{2}{3} (1 - D) C d \varepsilon^{pl} = \frac{2}{3} (1 - D) C d \bar{\varepsilon}^{pl} \mathbf{n}
\]  

(3.166)

The plasticity requires that the material satisfy a uniaxial-stress, plastic-strain and strain-rate relationship.

\[
q = (1 - D) \sigma_y
\]  

(3.167)

In any increment when plastic flow is occurring (which is determined by evaluating \( q \) based on the purely elastic response and finding that its value exceeds \((1 - D) \sigma_y\)), these equations must be integrated and solved for the state at the end of the increment. The integration is done by applying the backward Euler method to the flow rule (equation (3.164)) and hardening law (equation (3.166)), giving

\[
\Delta \mathbf{e}^{pl} = \Delta \bar{\varepsilon}^{pl} \mathbf{n}
\]  

(3.168)
\[ \Delta \alpha = \frac{2}{3}(1 - D)C \Delta e^\text{pl} = \frac{2}{3}(1 - D)C \Delta \bar{\varepsilon}^\text{pl} \mathbf{n} \] (3.169)

The backward Euler method is an unconditional stable and second-order accurate algorithm. Combining equation (3.168) with the deviatoric elasticity (equation (3.116)) and the integrated strain rate decomposition (equation (3.112)) gives

\[ S = 2(1 - D)G(e^\text{pl} \left| + \Delta e - \Delta \bar{\varepsilon}^\text{pl} \mathbf{n} \right) \] (3.170)

Rearranging equation (3.170), together with subtracting \( \alpha \) from both sides, this becomes,

\[ (S - \alpha) + \Delta \alpha = 2(1 - D)G\Delta \bar{\varepsilon}^\text{pl} \mathbf{n} = 2(1 - D)\hat{G}e - \alpha \]

where

\[ \hat{e} = e^\text{pl} \left| + \Delta e \right. \] (3.172)

\[ \alpha \left| = \alpha - \Delta \alpha \right. \] (3.173)

Then using the integrated hardening law together with the Mises definition of the flow direction \( \mathbf{n} \), this becomes

\[ \left( 1 + (1 - D)\frac{3G + C}{q} \Delta \bar{\varepsilon}^\text{pl} \right) (S - \alpha) = S^{\text{pr}} - \alpha \]

where

\[ S^{\text{pr}} = 2(1 - D)\hat{G}e \] (3.175)

With the help of equation (3.163), taking the inner product of equation (3.174) with itself gives

\[ q + (1 - D)(3G + C)\Delta \bar{\varepsilon}^\text{pl} = q^{\text{pr}} \]

where \( q^{\text{pr}} \) is the elastic predictor based on purely elastic behavior:
\[ q^{pr} = \sqrt{\frac{3}{2}} (S^{pr} - \sigma_i^t) : (S^{pr} - \alpha_i^t) \]  

Equation (3.177)

The Mises equivalent stress \( q \) must satisfy the uniaxial form defined in equation (3.167), so that, from equation (3.176),

\[ q^{pr} - (1 - D)(3G + C) \Delta \tilde{\varepsilon}^{pl} - (1 - D)\sigma_y = 0 \]

Equation (3.178)

where \( \Delta \tilde{\varepsilon}^{pl} \) can be solved by:

\[ \Delta \tilde{\varepsilon}^{pl} = \frac{q^{pr} - (1 - D)\sigma_y}{(1 - D)(3G + C)} \]

Equation (3.179)

Once \( \Delta \tilde{\varepsilon}^{pl} \) is known, the solution is fully defined.

Using equation (3.167):

\[ q = (1 - D)\sigma_y \]

Equation (3.180)

Using equation (3.174), equation (3.176) and equation (3.180):

\[ S - \alpha = \frac{S^{pr} - \alpha_i^t}{1 + \frac{3G + C}{\sigma_y} \Delta \tilde{\varepsilon}^{pl}} = (1 - D)\frac{\sigma_y}{q^{pr}} (S^{pr} - \alpha_i^t) \]

Equation (3.181)

Using equation (3.165) and equation (3.181):

\[ n = \frac{3}{2} \frac{S - \alpha}{(1 - D)\sigma_y} = \frac{3}{2} \frac{S^{pr} - \alpha_i^t}{q^{pr}} \]

Equation (3.182)

Using equation (3.168):

\[ \Delta e^{pl} = \Delta \tilde{\varepsilon}^{pl} n \]

Equation (3.183)

Using equation (3.169):

\[ \Delta \alpha = \frac{2}{3} (1 - D)C \Delta e^{pl} \]

Equation (3.184)

So, the back stress and deviatoric stress tensor can be determined as
\[ \alpha = \alpha_i + \Delta \alpha \]  \hspace{2cm} (3.185)

\[ S = (1 - D) \sigma_y \left( \frac{S^{pr} - \alpha}{q^{pr}} \right) + \alpha \]  \hspace{2cm} (3.186)

For cases where three direct strain components are provided by the kinematic solution, equation (3.115) defines:

\[ p = -(1 - D)K \varepsilon_{vol} = -(1 - D)K \varepsilon : \varepsilon \]  \hspace{2cm} (3.187)

So that the solution is then fully defined, and the material stiffness matrix can be derived without the need for matrix inversion as follows. Taking the variation of equation (3.176) with respect to all quantities at the end of the increment gives:

\[ \partial S = (1 - D) \sigma_y \partial \left( \frac{S^{pr} - \alpha}{q^{pr}} \right) + \partial \alpha \]  \hspace{2cm} (3.188)

From equation (3.175),

\[ \partial S^{pr} = 2(1 - D)G \partial \varepsilon \]  \hspace{2cm} (3.189)

and from equation (3.177),

\[ \partial q^{pr} = 3(1 - D)G \left( \frac{S^{pr} - \alpha}{q^{pr}} \right) : \partial \varepsilon = \frac{3G}{\sigma_y} (S - \alpha) : \partial \varepsilon \]  \hspace{2cm} (3.190)

where equation (3.186) has been used.

Then

\[ \partial \left( \frac{S^{pr} - \alpha}{q^{pr}} \right) = \frac{2(1 - D)G}{q^{pr}} \partial \varepsilon - \frac{3G}{(1 - D)\sigma_y q^{pr}} (S - \alpha) \otimes (S - \alpha) : \partial \varepsilon \]  \hspace{2cm} (3.191)

where equation (3.186) has been used.

From equation (3.179),
\[
\partial \varepsilon^{pl} = \frac{\partial q^p_{\tau}}{(1-D)(3G+C)} = \frac{3G}{(1-D)(3G+C)\sigma_y} - (S - \alpha) : \partial \varepsilon
\] (3.192)

From equation (3.182) and equation (3.183):
\[
\partial \varepsilon^{pl} = \frac{3}{2} \left[ \frac{3G}{(1-D)^2(3G+C)\sigma_y^2} (S - \alpha) \otimes (S - \alpha) : \partial \varepsilon + \Delta \varepsilon^{pl} \partial \left( \frac{S_{\tau}^{\tau} - \alpha_{\tau}^{\tau}}{q^{\tau\tau}} \right) \right]
\] (3.193)

where equation (3.186) and equation (3.192) have been used.

From equation (3.184) and equation (3.193):
\[
\partial \alpha = \frac{3GC}{(1-D)(3G+C)\sigma_y^2} (S - \alpha) \otimes (S - \alpha) : \partial \varepsilon + (1-D)C \Delta \varepsilon^{pl} \partial \left( \frac{S_{\tau}^{\tau} - \alpha_{\tau}^{\tau}}{q^{\tau\tau}} \right)
\] (3.194)

Combining these results with equation (3.188) gives:
\[
\partial S = \frac{2(1-D)^2 G(\sigma_y + C\Delta \varepsilon^{pl})}{q^{\tau\tau}} \partial \varepsilon - \frac{3G}{\sigma_y^2} \left[ \frac{(\sigma_y + C\Delta \varepsilon^{pl})}{q^{\tau\tau}} - \frac{C}{(1-D)(3G+C)} \right] (S - \alpha) \otimes (S - \alpha) : \partial \varepsilon
\] (3.195)

So, we have
\[
\partial S = [Q \Pi - R(S - \alpha) \otimes (S - \alpha)] : \partial \varepsilon
\] (3.196)

where
\[
Q = (1-D)^2 \frac{2G(\sigma_y + C\Delta \varepsilon^{pl})}{q^{\tau\tau}}
\] (3.197)
\[
R = \frac{3G}{\sigma_y^2} \left[ \frac{\sigma_y + C\Delta \varepsilon^{pl}}{q^{\tau\tau}} - \frac{C}{(1-D)(3G+C)} \right] = \frac{9G^2}{(3G+C)q^{\tau\tau} \sigma_y}
\] (3.198)

For all cases where three direct strains are defined by the kinematic solution the material
stiffness is completed by (from equation (3.115)):
\[
\partial p = -(1-D)KI : \partial \varepsilon
\] (3.199)

So that, since (from equation (3.108)):  

98
\[ \sigma = S - pI \] (3.200)

and (from equation (3.106)):

\[ \hat{\sigma} \hat{e} = \hat{\sigma} e = \left( \mathbf{I} - \frac{1}{3} \mathbf{I} \otimes \mathbf{I} \right) : \hat{\sigma} e \] (3.201)

Because

\[ \sigma = \hat{e} + \epsilon^{pl} \mid \epsilon, \] (3.202)

we have

\[ \hat{\sigma} = \left[ ((1 - D)K - \frac{1}{2} Q) \mathbf{I} \otimes \mathbf{I} + Q \mathbf{I} - R(S - a) \otimes (S - a) \right] \hat{\epsilon} e \] (3.203)

Equation (3.203) can also be written in alternate form:

\[ \Delta \sigma_{ij} = \lambda^* \delta_{ij} \Delta \hat{\epsilon}_{ij} + 2 \mu^* \Delta \hat{\epsilon}_{ij} + \left( \frac{(1 - D)C}{1 + C/3G} - 3 \mu^* \right) \eta_{ij} \eta_{ij} \Delta \hat{\epsilon}_{ij} \] (3.204)

where

\[ \mu^* = (1 - D)^2 \frac{G \epsilon + \epsilon \Delta \epsilon^{pl}}{q^{pr}} \] (3.205)

\[ \lambda^* = (1 - D)K - \frac{2}{3} \mu^* \] (3.206)

\[ \eta_{ij} = (S_{ij}^{pr} - \alpha_{ij}) / q^{pr} \] (3.207)

From equation (3.175), equation (3.186), equation (3.187) and equation (3.200), we have

\[ \sigma_{ij} = \alpha_{ij} + \eta_{ij} \sigma_{jj} + \frac{1}{3} \delta_{ij} \sigma_{kk}^{pr} \] (3.208)
CHAPTER 4

Damage Coupled Constitutive Model of Particulate Composites

4.1 Introduction

The application and estimation of the effective mechanical properties of random heterogeneous multiphase materials are of great interest to researchers and engineers in many science and engineering disciplines. There are many different methods and tools that can be used to deliver the macroscopic constitutive response of heterogeneous materials from a local description of the microstructural behavior. In the development of the homogenization procedures for heterogeneous materials, we have to define both the homogenization step itself (from local variables to overall ones) and the often more complicated localization step (from overall controlled quantities to the corresponding local ones). Numerous papers on the determination of effective thermomechanical properties of heterogeneous materials have been published. However, up to now no formula has been derived which is theoretically well founded and fits experimental results for a whole range of volume concentrations.

Based on generalizations of the Eshelby method (Eshelby, 1957), a novel micromechanical framework has been proposed by Ju and Chen (1994a, 1994b) to investigate the effective mechanical properties of elastic multiphase composites containing many randomly dispersed ellipsoidal inhomogeneities with perfect bonding.
Within the context of the representative volume element (REV), four governing micromechanical ensemble-volume averaged field equations are presented to relate ensemble-volume averaged stresses, strains, volume fractions, eigenstrains, particle shapes and orientations, and elastic properties of constituent phases of the particulate composites. The various micromechanical models can be developed based on the proposed ensemble-volume averaged constitutive equations. In Ju and Tseng (1996), a formulation combining a micromechanical interaction approach and the continuum plasticity is proposed to predict effective elastoplastic behavior of two-phase particulate composite containing many randomly dispersed elastic spherical inhomogeneities. Explicit pairwise interparticle interactions are considered in both the elastic and plastic responses. Furthermore, the ensemble-volume averaging procedure is employed and the formulation is of complete second order.

Let us consider a perfectly bonded two-phase composite consisting of an elastic matrix (phase 0) with bulk modulus $k_0$ and shear modulus $\mu_0$, and randomly dispersed elastic spherical particles (phase 1) with bulk modulus $k_1$ and shear modulus $\mu_1$. The effective bulk modulus $k^*$ and shear modulus $\mu^*$ for this two-phase composite was explicitly expressed by Ju and Chen (1994a, 1994b). The noninteracting solutions were obtained by neglecting the inter-particle interaction effects (Ju and Chen, 1994a).

\[
k^* = k_0 \left\{ 1 + \frac{3(1-\nu_0)(k_1-k_0)\phi}{3(1-\nu_0)k_0 + (1-\phi)(1+\nu_0)(k_1-k_0)} \right\} \tag{4.1}
\]

\[
\mu^* = \mu_0 \left\{ 1 + \frac{15(1-\nu_0)(\mu_1-\mu_0)\phi}{15(1-\nu_0)\mu_0 + (1-\phi)(8-10\nu_0)(\mu_1-\mu_0)} \right\} \tag{4.2}
\]
where $\phi$ is the particle volume fraction, $v_0$ is the Poisson’s ratio of the matrix. It is shown that the classical Hashin-Shtrikman’s bounds (1963), Walpole’s bounds (1966), and Willis’ bounds (1991) for isotropic or anisotropic elastic multiphase composites are related to the noninteracting solutions. Further, it is demonstrated that the Mori-Tanaka method (1973) coincides with the Hashin-Shtrikman bounds and the noninteracting micromechanical model in some cases.

If the effects due to inter-particle interactions are included for the two-phase elastic composites with randomly located spherical particles, the solutions for the effective bulk modulus $k_*$ and shear modulus $\mu_*$ are (Ju and Chen, 1994b):

$$k_* = k_0 \left\{ 1 + \frac{30(1-v_0)\phi(3\gamma_1 + 2\gamma_2)}{3\alpha + 2\beta - 10(1+v_0)\phi(3\gamma_1 + 2\gamma_2)} \right\}$$

$$\mu_* = \mu_0 \left\{ 1 + \frac{30(1-v_0)\phi\gamma_2}{\beta - 4(4-5v_0)\phi\gamma_2} \right\}$$

with

$$\alpha = 2(5v_0 - 1) + 10(1-v_0)\left\{ \frac{k_0}{k_i - k_0} - \frac{\mu_0}{\mu_i - \mu_0} \right\}$$

$$\beta = 2(4-5v_0) + 15(1-v_0)\frac{\mu_0}{\mu_i - \mu_0}$$

and

$$\gamma_1 = \frac{5\phi}{8\beta^2} \left\{ (13-14v_0)v_0 - \frac{8\alpha}{3\alpha + 2\beta}(1-2v_0)(1+v_0) \right\}$$

$$\gamma_2 = \frac{1}{2} + \frac{5\phi}{16\beta^2} \left\{ (25-34v_0 + 22v_0^2) - \frac{6\alpha}{3\alpha + 2\beta}(1-2v_0)(1+v_0) \right\}$$
Alternatively, the effective Young’s modulus $E_*$ and Poisson’s ratio $\nu_*$ of particulate composites are easily obtained through the following relationship:

$$
E_* = \frac{9k_\mu}{3k_\mu + \mu} 
$$

(4.9)

$$
\nu_* = \frac{3k_\mu - 2\mu}{6k_\mu + 2\mu} 
$$

(4.10)

In order to further assess the validity of the proposed Ju and Chen’s method, we now compare the analytical predictions with the available experimental data on the particulate composite prepared using lightly cross-linked poly-methyl methacrylate (PMMA) filled with alumina trihydrate (ATH). All particles are assumed to be spherical and both the matrix and the particle are isotropic elastic. The material properties involved are as follows:

ATH: $E_i = 70$ GPa, $\nu_i = 0.24$

PMMA: $E_0 = 3.5$ GPa, $\nu_0 = 0.31$

Particle volume fraction: $\phi = 0.48$

Experimental mean value of Young’s modulus for this composite is about 10.2 GPa at room temperature. Figure 4.1 shows the comparisons among the analytical solution (including pairwise interacting solution and noninteracting solution) and experimental results. It is observed that agreement between the pairwise interacting prediction and experimental data is very good for the effective Young’s modulus. Based on the foregoing preliminary analytical and experimental comparisons, it appears that the Ju and Chen’s analytical micromechanical approach offers a simple, approximate, yet
sufficiently accurate framework for the prediction of effective elastic moduli of two-phase composites.

![Diagram showing effective Young's modulus as a function of particle volume fraction]

Figure 4.1 Effective Young’s modulus as a function of particle volume fraction

As we have known, particulate composites consist of bulk matrix, filler-particles, and interfacial transition zone around particles, which often have very different properties such as coefficient of thermal expansion (CTE) and stiffness. So it is no wonder that within the particulate composite microstructure there exists microstress associated with the coefficient of the thermal expansion (CTE) mismatch between the matrix and the particles. For the composite prepared using lightly cross-linked poly-methyl methacrylate (PMMA) filled with alumina trihydrate (ATH), these microstresses can be imaged using the fact that PMMA is stress optically birefringent. The microstresses imaged using this technique are indeed due to CTE mismatch as they dissipate at temperatures close to the
glass transition temperature $T_g$ of the PMMA. These stresses can be quantified by calculation or by direct measurement and are of the order between 15% and 75% of the tensile strength of the composite. Therefore the thermal stress associated with the CTE mismatch between the matrix and particles is an important factor for the failure of particulate composite subjected to thermomechanical loads. But the original micromechanical model of Ju and Chen (1994a, 1994b), Ju and Tseng (1996), can’t account for the effects of the linear thermal expansion coefficient mismatch. In this dissertation, we expanded Ju and Chen’s micromechanical model to incorporate the effects of CTE mismatch between the matrix and particles.

It is well known that the bonding conditions between the matrix and particles have significant effects on the behavior of the composite. In order to directly use the current micromechanical field equation (Mura, 1987) and also consider the CTE mismatch and bonding conditions between matrix and particles, composites are treated as two distinct phases, namely the bulk matrix and the equivalent particles-interphase assembly in this work.

4.2 Ensemble-Volume Averaged Micromechanical Field Equations

In this section, the procedure of Ju and Chen (1994a) was still followed to incorporate the CTE mismatch between the matrix and the particle into the model. To obtain effective constitutive equations and properties of random heterogeneous composites, one typically performs the ensemble-volume averaging process within a mesoscopic representative volume element (RVE). The volume-averaged stress tensor is defined as
\[
\bar{\sigma} = \frac{1}{V} \int_V \sigma(x) \, dx = \frac{1}{V} \left[ \int_{V_0} \sigma(x) \, dx + \sum_{q=1}^{n} \int_{V_{0q}} \sigma(x) \, dx \right] = \frac{1}{V} \left[ V_0 \bar{\sigma}_0 + \sum_{q=1}^{n} V_q \bar{\sigma}_q \right] \tag{4.11}
\]

where \( V \) is the volume of a RVE, \( V_0 \) is the volume of the matrix, \( V_q \) is the volume of the \( q^{th} \) phase particles, and \( n \) denotes the number of particulate phases of different material properties (excluding the matrix).

Similarly, the volume-averaged strain tensor is defined as

\[
\bar{\varepsilon} = \frac{1}{V} \int_V \varepsilon(x) \, dx = \frac{1}{V} \left[ \int_{V_0} \varepsilon(x) \, dx + \sum_{q=1}^{n} \int_{V_{0q}} \varepsilon(x) \, dx \right] = \frac{1}{V} \left[ V_0 \bar{\varepsilon}_0 + \sum_{q=1}^{n} V_q \bar{\varepsilon}_q \right] \tag{4.12}
\]

According to Eshelby’s equivalence principle, the perturbed strain field \( \varepsilon'(x) \) induced by inhomogeneities can be related to specified eigenstrain \( \varepsilon^*(x) \) by replacing the inhomogeneities with the matrix material. Sometimes the inhomogeneities may also involve its own eigenstrain caused by, for example phase transformation, precipitation, plastic deformation, or CTE mismatch between different constituents of the composites. However, it is not necessary to attribute the eigenstrain to any specific source. Then the total perturbed stress is the sum of the two parts, one caused by the inhomogeneity, and the other one is the eigenstress caused by eigenstrain. For the domain of the \( q^{th} \)-phase particles with elastic stiffness tensor \( C_q \), we have (Mura, 1987)

\[
C_q : [\varepsilon^0 + \varepsilon'(x) - \varepsilon_q^*(x)] = C_0 : [\varepsilon^0 + \varepsilon'(x) - \varepsilon_q^*(x) - \varepsilon_q^*(x)] \tag{4.13}
\]

where \( C_0 \) is the stiffness tensor of the matrix and \( \varepsilon^0 \) is the uniform elastic strain field induced by far-field loads for a homogeneous matrix material only. \( \varepsilon_q^* \) is its own eigenstrain associated with the \( q^{th} \) particle. \( \varepsilon_q^* \) is the fictitious equivalent eigenstrain by
replacing the \( q^{th} \) particles with the matrix material. \( \epsilon'(x) \) is the perturbed strain due to distributed eigenstrain \( \epsilon^* \) and \( \epsilon^r \) associated with all particles in the RVE. And the matrix stress is given by

\[
\sigma^0 = C_0 : \epsilon^0
\]  

(4.14)

The strain at any point within an RVE is decomposed into two parts, the uniform strain and the perturbed strain due to the distributed eigenstrain. It is emphasized that the eigenstrain \( \epsilon^* \) and \( \epsilon^r \) are nonzero in the particle domain and zero in the matrix domain, respectively. In particular, in accordance with Eshelby, the perturbed strain field induced by all the distributed eigenstrain \( \epsilon^* \) and \( \epsilon^r \) can be expressed as (Mura, 1987):

\[
\epsilon'(x) = \int V(x, x') : \left[ \epsilon^r(x') + \epsilon^*(x') \right] dV'
\]  

(4.15)

where \( x, x' \in V \), and \( G \) is the Green’s function in a linear elastic homogeneous matrix. For a linear elastic isotropic matrix, the fourth rank tensor Green’s function is given (Ju and Chen, 1994a)

\[
G_{ijkl}(x - x') = \frac{1}{8\pi(1 - v_0)r^3} F_{ijkl} (-15, 3v_0, 3, 3 - 6v_0, -1 + 2v_0, 1 - 2v_0)
\]  

(4.16)

where \( r \equiv x - x', r \equiv |r| \), and \( v_0 \) is the Poisson’s ratio of the matrix. The components of the fourth rank tensor \( F \) are defined by

\[
F_{ijkl}(B_m) = B_1n_in_jn_kn_l + B_2(\delta_{ik}n_jn_l + \delta_{jl}n_jn_k + \delta_{jk}n_in_l + \delta_{ji}n_jn_k) + B_3\delta_{ik}n_jn_k + B_4\delta_{jl}n_jn_l + B_5\delta_{ik}n_jn_l + B_6(\delta_{ij}n_k + \delta_{jk}n_i + \delta_{jk}n_i)
\]  

(4.17)

with the unit normal vector \( n \equiv r/r \) and index \( m = 1 \) to \( 6 \).

From equations (4.13) and (4.15), we arrive at
\[-A_q : \varepsilon_q^* (x) = \varepsilon^0 - \varepsilon_q^T (x) + \int_V G(x - x') \left[ \varepsilon_T (x') + \varepsilon^* (x') \right] dx' \quad x' \in V \quad (4.18)\]

where

\[A_q = (C_q - C_0)^{-1} \cdot C_0 \quad (4.19)\]

Furthermore, the total local strain field \(\varepsilon (x)\) can be expressed as

\[\varepsilon (x) = \varepsilon^0 + \varepsilon' (x) = \varepsilon^0 + \int_V G(x - x') \left[ \varepsilon_T (x') + \varepsilon^* (x') \right] dx' \quad (4.20)\]

Using the renormalization procedure employed in (Ju and Chen, 1994a), the volume-averaged strain tensor is given by:

\[\bar{\varepsilon} = \varepsilon^0 + \frac{1}{V} \int_V \int_V G(x - x') \left[ \varepsilon_T (x') + \varepsilon^* (x') \right] dx'dx = \varepsilon^0 + s : \left[ \sum_{q=1}^n \phi_q (\bar{\varepsilon}_q^T + \bar{\varepsilon}_q^*) \right] \quad (4.21)\]

where \(s\) is a constant tensor for unidirectionally aligned and similarly ellipsoidal particles. If the linear elastic matrix material is isotropic and all inclusions are spherical, then the \(s\) takes the form of the Eshelby tensor \(S\):

\[S_{ijkl} = \frac{1}{15(1 - \nu_0)} \left[ (5\nu_0 - 1) \delta_{ij} \delta_{kl} + (4 - 5\nu_0) (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \right] \quad (4.22)\]

where \(\delta_{ij}\) signifies the Kronecker delta.

Similarly, using equations (4.11), (4.12) & (4.13), the ensemble-volume averaged stress field can be recast as:

\[\bar{\sigma} = \frac{1}{V} \left[ \int_{V_0} C_0 : \varepsilon_0 dx + \sum_{q=1}^n \int_{V_q} C_0 : \left[ \varepsilon (x) - \varepsilon_q^T - \varepsilon_q^* \right] dx \right] \]

\[= \frac{1}{V} \left[ V_0 C_0 : \varepsilon_0 + \sum_{q=1}^n V_q C_0 : \left[ \bar{\varepsilon}_q - \bar{\varepsilon}_q^T - \bar{\varepsilon}_q^* \right] \right] = C_0 : \left[ \bar{\varepsilon} - \sum_{q=1}^n \phi_q (\bar{\varepsilon}_q^T + \bar{\varepsilon}_q^*) \right] \quad (4.23)\]
The effective elastic properties can be obtained, in principle, from equations (4.18), (4.21) and (4.23) since the variables are $\bar{\sigma}, \bar{\varepsilon}, \varepsilon^0, \bar{\varepsilon}'$. In essence, one needs to solve the relation between $\bar{\varepsilon}$ and $\bar{\varepsilon}'$, which involves the solution of the integral equation (4.18). $\bar{\varepsilon}'$ depends on inter-particle interactions, particle-matrix interactions and microstructure (i.e. particle sizes, orientation, shapes, volume fractions, locations, configurations, and probability functions) of a composite system. For randomly dispersed particles, one needs to obtain the ensemble-volume averaged relation between $\bar{\varepsilon}$ and $\bar{\varepsilon}'$ by averaging all possible solutions of the integral equation (4.18) for any particle configurations generated according to specified probability functions.

Taking the ensemble-volume average of equation (4.18) over all $q^{th}$-phase particles, we obtain:

$$-A_q : \bar{\varepsilon}' = \varepsilon^0 - \varepsilon'^0 + \bar{\varepsilon}'$$

(4.24)

where

$$\bar{\varepsilon}' = \frac{1}{V_q} \int \int G(\mathbf{x} - \mathbf{x}')\left[\varepsilon'^0(\mathbf{x}') + \varepsilon^*(\mathbf{x}')\right]d\mathbf{x}'d\mathbf{x}$$

(4.25)

If all particles in the $q^{th}$-phase have the same ellipsoidal shape and orientation, then $\bar{\varepsilon}'$ can be recast as

$$\bar{\varepsilon}' = \bar{\varepsilon}^{ip}_q + S_q : \left(\bar{\varepsilon}' + \bar{\varepsilon}'\right)$$

(4.26)

with

$$\bar{\varepsilon}^{ip}_q = \frac{1}{V_q} \sum_{i=1}^{N_q} \int_{\Omega_q} \int_{\Omega_q'} G(\mathbf{x} - \mathbf{x}')\left[\varepsilon'^0(\mathbf{x}') + \varepsilon^*(\mathbf{x}')\right]d\mathbf{x}'d\mathbf{x}$$

(4.27)
representing the inter-particle interaction effects. Where $\Omega_q$ is the domain of the $q^{th}$ particle in the $q^{th}$ phase domain $V_q$ and $N_q$ is the number of the phase $q$ particles dispersed in $V$. $S_q$ is the Eshelby tensor associated the $q^{th}$ particle.

From equations (4.24) and (4.26), we arrive at

$$
\left(-A_q - S_q\right) : \tilde{\varepsilon}_q^* = \varepsilon^0 - \varepsilon^T + S_q : \varepsilon^T + \varepsilon_q^p
$$

(4.28)

In summary, the three basic governing micromechanical ensemble-volume averaged field equations are recapitulated as follows:

$$
\bar{\sigma} = C_0 : \left[ \bar{\varepsilon} - \sum_{q=1}^n \phi_q \left( \tilde{\varepsilon}_q^* + \tilde{\varepsilon}_q^T \right) \right]
$$

(4.29)

$$
\bar{\varepsilon} = \varepsilon^0 + \sum_{q=1}^n \phi_q s : \left( \tilde{\varepsilon}_q^T + \tilde{\varepsilon}_q^* \right)
$$

(4.30)

$$
-(A_q + S_q) : \tilde{\varepsilon}_q^* = \varepsilon^0 - \varepsilon^T + S_q : \varepsilon_q^T + \varepsilon_q^p
$$

(4.31)

To actually solve equations (4.29), (4.30) and (4.31) and obtain effective elastic properties of composite, it is essential to express the $q^{th}$-phase average eigenstrain $\tilde{\varepsilon}_q^*$ in terms of the average strain $\bar{\varepsilon}$. Namely, one has to solve the integral equation (4.18) exactly for each phase, which involves details of random microstructure.

### 4.3 Noninteracting Solution for Two-Phase Composites

Let us consider a perfectly bonded two-phase composite consisting of a viscoplastic matrix (phase 0) with elastic bulk modulus $k_0$ and elastic shear modulus $\mu_0$, and randomly dispersed elastic spherical particles (phase 1) with bulk modulus $k_1$ and shear modulus $\mu_1$. For simplicity, the von Mises yield criterion is assumed for the matrix
Extension of the present framework to the general yield criterion and the general hardening law, however, is straightforward. Accordingly, at any matrix material point, the stress $\sigma$ and the equivalent plastic strain $e^p$ must satisfy the following yield function

$$ F(\sigma, e^p) = \sqrt{H(\sigma)} - K(e^p) $$

(4.32)

where $K(e^p)$ is the isotropic hardening function of the matrix-only material. Furthermore, $H(\sigma)$ signifies the square of the deviatoric stress norm,

$$ H(\sigma) = \sigma : I_d : \sigma $$

(4.33)

where $I_d$ denotes the deviatoric part of the fourth rank identity tensor.

$$ (I_d)_{ijkl} = -\frac{1}{3} \delta_{ij} \delta_{kl} + \frac{1}{2} \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) $$

(4.34)

In order to solve the elastoplastic response exactly, the stress at any local point has to be known and used to determine the plastic response through the local yield criterion for all possible configurations. This approach is in general infeasible due to the complexity of the statistical and microstructural information. Therefore, a framework in which an ensemble averaged yield criterion is constructed for the entire composite is used (Ju and Tseng, 1996).

### 4.3.1. Average Stress Norm in Matrix

Following Ju and Chen (1994a), the total stress $\sigma(x)$ at any point $x$ in the matrix is given by the superposition of the far-field stress $\sigma_0$ and the perturbed stress $\sigma'$ induced by the particles:

$$ \sigma(x) = \sigma_0 + \sigma'(x) $$

(4.35)
According the Eshelby theory, the perturbed stress $\sigma'$ at any point in the matrix due to the presence of the particles can be written as:

$$\sigma'(x) = C_0 \cdot \int \mathbf{G}(x - x') \cdot \left[ \epsilon' + \epsilon''(x') \right] dx'$$  \hspace{1cm} (4.36)

where $\epsilon''(x')$ denotes the fictitious elastic eigenstrain in the particle induced by replacing the inhomogeneities with the matrix material. $\epsilon'$ is its own eigenstrain associated with the inhomogeneities. Assuming $\epsilon'$ is uniform in the particles, $\mathbf{G}(x - x')$ is the fourth rank tensor of the Green’s function defined by equation (4.16).

According the Eshelby theory, the eigenstrain $\epsilon''(x')$ in a single ellipsoidal inclusion is uniform for the interior points of an isolated (noninteracting) inclusion. Therefore, the perturbed stress for any matrix point $x$ due to a typical isolated inhomogeneity centered at $x_i$ takes the form

$$\sigma'(x|x_i) = \left[ C_0 \cdot \mathbf{G}(x - x_i) \right] : \left( \epsilon' + \epsilon'' \right)$$  \hspace{1cm} (4.37)

where

$$\mathbf{G}(x - x_i) = \int_{\Omega_i} \mathbf{G}(x - x') dx' \text{ for } x \not\in \Omega_i$$  \hspace{1cm} (4.38)

here $\Omega_i$ is the particle domain centered at $x_i$. Alternatively we can derive

$$\mathbf{G}(x - x_i) = \frac{\rho^3}{30(1 - \nu_o)} \left( \mathbf{H}^1 + \rho^2 \mathbf{H}^2 \right)$$  \hspace{1cm} (4.39)

where the components of $\mathbf{H}^1$ and $\mathbf{H}^2$ are given by:

$$H^1_{ijkl}(r) = 5F_{ijkl} \left( -15, 3v_0, 3, 3 - 6v_0, -1 + 2v_0, 1 - 2v_0 \right)$$  \hspace{1cm} (4.40)

$$H^2_{ijkl}(r) = 3F_{ijkl} \left( 35, -5, -5, -5, 1, 1 \right)$$  \hspace{1cm} (4.41)
where \( \mathbf{r} \equiv \mathbf{x} - \mathbf{x}_1, r \equiv |\mathbf{r}|, \ \rho = a/r \) and \( a \) is the radius of a spherical particle. The components of the fourth rank tensor \( \mathbf{F} \) are given by equation (4.17). In equation (4.37), \( \varepsilon^{\nu} \) denotes the solution of the eigenstrain \( \varepsilon^\nu \) for the single inclusion problem, which is given (from equation (4.31) when \( \varepsilon^\nu \) is dropped):

\[
\varepsilon^{\nu} = - \left( \mathbf{A} + \mathbf{S} \right)^{-1} \cdot \varepsilon^\nu + \left( \mathbf{A} + \mathbf{S} \right)^{-1} \cdot \left( \mathbf{I} - \mathbf{S} \right) \cdot \varepsilon^{\nu} \]  

(4.42)

where

\[
\mathbf{A} = \left( \mathbf{C}_1 - \mathbf{C}_0 \right)^{-1} \cdot \mathbf{C}_0 \]  

(4.43)

Similarly with Ju and Tseng (1997), we denote by \( H\left(\mathbf{x}|\phi\right) \) the square of the current stress norm at the local point \( \mathbf{x} \), which determines the plastic strain in a particulate composite for a given phase configuration \( \phi \). Since there is no plastic strain in the elastic particles or voids, \( H\left(\mathbf{x}|\phi\right) \) can be written as

\[
H\left(\mathbf{x}|\phi\right) = \begin{cases} \mathbf{\sigma}\left(\mathbf{x}|\phi\right) : \mathbf{I}_x : \mathbf{\sigma}\left(\mathbf{x}|\phi\right) & \mathbf{x} \text{ in the matrix} \\ 0 & \text{otherwise} \end{cases} 
\]  

(4.44)

In addition, \( \langle H \rangle_m\left(\mathbf{x}\right) \) is defined as the ensemble average of \( H\left(\mathbf{x}|\phi\right) \) over all possible realizations where \( \mathbf{x} \) is in the matrix phase. Matrix point receives the perturbations from particles. Therefore, the ensemble-average stress norm for any matrix point \( \mathbf{x} \) can be evaluated by collecting and summing up all the current stress norm perturbations produced by any typical particle centered at \( \mathbf{x}_i \) in the particle domain and averaging over all possible locations of \( \mathbf{x}_i \), namely

\[
\langle H \rangle_m\left(\mathbf{x}\right) = H^\nu + \int_{x_1} \left\{ H\left(\mathbf{x}|\mathbf{x}_i\right) - H^\nu \right\} P\left(\mathbf{x}_i\right) d\mathbf{x}_i
\]  

(4.45)
for \( \mathbf{x} \) in the matrix. Here \( a \) is the radius of the particles, \( P(\mathbf{x}) \) denotes the probability density functions for finding a particle centered at \( \mathbf{x} \), and \( H_0 \) corresponds to the far-field stress norm in the matrix:

\[
H^0 = \sigma^0 : \mathbf{I}_d : \sigma^0
\]  
(4.46)

where \( \mathbf{I}_d \) signifies the deviatoric part of the forth rank identity tensor.

Assuming that \( P(\mathbf{x}) \) is statistically homogeneous, isotropic and uniform, and \( P(\mathbf{x}) \) takes the form

\[
P(\mathbf{x}) = \frac{N}{V}
\]  
(47)

where \( N \) is the total number of particles dispersed in volume \( V \). According to the assumption of statistical isotropy and uniformity, equation (4.45) can be recast into a more convenient form:

\[
\left< H \right>_m(\mathbf{x}) \approx H^0 + \frac{N}{V} \int_{r \leq a} d\mathbf{r} \int_{d(r)} \{ H(\mathbf{r}) - H^0 \} dA
\]  
(4.48)

With the help of equations (4.35), (4.37), (4.44) and (4.46), plus using the following identities,

\[
\int_{d(\mathbf{r})} n_i n_j dA = \frac{4\pi r^2}{3} \delta_{ij}
\]  
(4.49)

\[
\int_{d(\mathbf{r})} n_i n_j n_k n_l dA = \frac{4\pi r^2}{15} \left( \delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right)
\]  
(4.50)

\[
\int_{r \leq a} d\mathbf{r} \int_{d(\mathbf{r})} H^1(\mathbf{r}) dA = 0
\]  
(4.51)

\[
\int_{r \leq a} d\mathbf{r} \int_{d(\mathbf{r})} H^2(\mathbf{r}) dA = 0
\]  
(4.52)
\[ \int_{r_{\text{in}}} dr \int_{d(r)} G(r) dA = 0 \]  

(4.53)

equation (4.48) can be recast as:

\[
\langle H \rangle_m (x) = H_0^0 + N \int_{r_{\text{in}}} dr \int_{d(r)} [\sigma'(x) : I : \sigma'(x)] dA
\]

(4.54)

After some lengthy yet straightforward derivations, we obtain the ensemble-averaged current stress norm at any matrix point \( x \) as:

\[
\langle H \rangle_m (x) = \sigma^0 : T : \sigma^0 + \sigma^T : T^* : \sigma^T - 2 \sigma^0 : T^* : \sigma^T
\]

(4.55)

where

\[
\sigma^T = A C_1 : \varepsilon^T
\]

(4.56)

The components of the positive definite fourth-rank tensor \( T \) and \( T^* \) read

\[
T_{ijkl} = T_1 \delta_{ij} \delta_{kl} + T_2 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right)
\]

(4.57)

\[
T^*_{ijkl} = T_1^* \delta_{ij} \delta_{kl} + T_2^* \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right)
\]

(4.58)

with

\[
3 T_1 + 2 T_2 = 200 (1 - 2 \nu_0)^2 \frac{\phi}{(3 \alpha + 2 \beta)^2}
\]

(4.59)

\[
T_2 = \frac{1}{2} + (23 - 50 \nu_0 + 35 \nu_0^2) \frac{\phi}{\beta^2}
\]

(4.60)

\[
3 T_1^* + 2 T_2^* = 200 (1 - 2 \nu_0)^2 \frac{\phi}{(3 \alpha + 2 \beta)^2}
\]

(4.61)

\[
T_2^* = (23 - 50 \nu_0 + 35 \nu_0^2) \frac{\phi}{\beta^2}
\]

(4.62)

\( \alpha \) and \( \beta \) are given by equations (4.5) and (4.6) \( \phi \) is the particle volume fraction.
The ensemble-averaged current stress norm at a matrix point must be established in terms of the macroscopic stress $\bar{\sigma}$ in order to express the effective loading function in terms of the macroscopic stress. In the special case of uniform dispersions of identical elastic spheres in a homogeneous matrix, the macroscopic stress and the far-filed stress take the form,

$$\bar{\sigma} = C_0 : \left[ \bar{\varepsilon} - \phi \left( \bar{\varepsilon}^T + \bar{\varepsilon}^0 \right) \right]$$  \hspace{1cm} (4.63)

$$\sigma^0 = C_0 : \left[ \bar{\varepsilon} - \phi S : \left( \bar{\varepsilon}^T + \bar{\varepsilon}^0 \right) \right]$$  \hspace{1cm} (4.64)

Using equations (4.63), (4.64) & (4.42), the relation between the far-field stress $\sigma^0$ and the macroscopic stress $\bar{\sigma}$ takes the form

$$\bar{\sigma} = P : \sigma^0 - Q : \sigma^r$$  \hspace{1cm} (4.65)

where

$$P = I + \phi (I - S)(A + S)^{-1}$$  \hspace{1cm} (4.66)

$$Q = \phi (I - S)(A + S)^{-1}$$  \hspace{1cm} (4.67)

with the components of $P$ and $Q$ are

$$P_{ijkl} = \delta_{ij} \delta_{kl} + P_1 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right)$$  \hspace{1cm} (4.68)

$$Q_{ijkl} = Q_1 \delta_{ij} \delta_{kl} + Q_2 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right)$$  \hspace{1cm} (4.69)

where

$$3P_1 + 2P_2 = a\phi + 1$$  \hspace{1cm} (4.70)

$$P_2 = \frac{1}{2} \left( b\phi + 1 \right)$$  \hspace{1cm} (4.71)

$$3Q_1 + 2Q_2 = a\phi$$  \hspace{1cm} (4.72)
\begin{align}
Q_2 &= \frac{1}{2} b \phi \\
a &= \frac{20(1 - 2v_o)}{3\alpha + 2\beta} \\
b &= \frac{(7 - 5v_o)}{\beta}
\end{align}

With the help of equation (4.65), we arrive at the alternative expression for the ensemble-averaged current stress norm in a matrix point \( \mathbf{x} \) as:

\[ \langle H \rangle_{\alpha}(\mathbf{x}) = \mathbf{\bar{\sigma}} : \mathbf{T} : \mathbf{\bar{\sigma}} + 2\mathbf{\bar{\sigma}} : \mathbf{T}^\prime : \mathbf{\bar{\sigma}}^\prime + \mathbf{\bar{\sigma}}^\prime : \mathbf{T}^{\prime\prime} : \mathbf{\bar{\sigma}}^{\prime\prime} \]  

(4.76)

where the positive definite fourth-rank tensor \( \mathbf{T} \), \( \mathbf{T}^\prime \), and \( \mathbf{T}^{\prime\prime} \) are defined as

\[ \mathbf{T} = \left( \mathbf{P}^{-1} \right)^T \cdot \mathbf{T} \cdot \mathbf{P}^{-1} \]  

(4.77)

\[ \mathbf{T}^\prime = \left( \mathbf{P}^{-1} \right)^T \cdot \mathbf{T} \cdot \mathbf{P}^{-1} \cdot \mathbf{Q} - \mathbf{T}^\prime \cdot \mathbf{P}^{-1} \]  

(4.78)

\[ \mathbf{T}^{\prime\prime} = \left( \mathbf{P}^{-1} \cdot \mathbf{Q} \right)^T \cdot \mathbf{T} \cdot \left( \mathbf{P}^{-1} \cdot \mathbf{Q} \right) + \mathbf{T}^\prime - 2\mathbf{T}^\prime \cdot \left( \mathbf{P}^{-1} \cdot \mathbf{Q} \right) \]  

(4.79)

where the components of \( \mathbf{T} \), \( \mathbf{T}^\prime \), and \( \mathbf{T}^{\prime\prime} \) are

\[ \bar{T}_{ijkl} = \bar{T}_{ijkl} + \bar{T} \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \]  

(4.80)

\[ \bar{T}^\prime_{ijkl} = \bar{T}^\prime_{ijkl} + \bar{T}^\prime \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \]  

(4.81)

\[ \bar{T}^{\prime\prime}_{ijkl} = \bar{T}^{\prime\prime}_{ijkl} + \bar{T}^{\prime\prime} \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \]  

(4.82)

with

\[ 3\bar{T} + 2\bar{T}^\prime = \frac{3T_1 + 2T_2}{(a\phi + 1)^2} \]  

(4.83)

\[ \bar{T}_2 = \frac{T_2}{(b\phi + 1)^2} \]  

(4.84)
Because $\sigma^T = \mathbf{A}C_1 : \mathbf{e}^T$ is spherical stress, so equation (4.76) of the ensemble-averaged loading function can be simplified as

$$3T_1^{**} + 2T_2^{**} = \frac{3T_1 + 2T_2}{(a\phi + 1)^2}$$

(4.85)

$$T_2^{**} = \frac{T_2}{(b\phi + 1)^2} + \frac{1}{2(b\phi + 1)}$$

(4.86)

$$3T_1^{***} + 2T_2^{***} = \frac{3T_1 + 2T_2}{(a\phi + 1)^3}$$

(4.87)

$$T_2^{***} = \frac{T_2}{(b\phi + 1)^2} + \frac{b\phi - 1}{2(b\phi + 1)}$$

(4.88)

It should be noted that the effective loading function is pressure dependent now and not of the von-Mises type any more. So the particles have significant effects on the viscoplastic behavior of the matrix materials. Plastic yielding and plastic flow occur only in the matrix. Regarded the two-phase composite as plastic overall when the ensemble-volume averaged current stress norm in the matrix reaches a certain level. The magnitude of the current equivalent stress norm is utilized to determine the possible viscoplastic strain for any point in the composite.

### 4.3.2 Average Stress in Particles

If the particle interaction for two-phase composite was ignored, equation (4.30) becomes

$$\bar{\epsilon} = \bar{\epsilon}^0 + \phi S : (\bar{\sigma}^T + \bar{\sigma}^{*0})$$

(4.90)
With the noninteracting solution \( \varepsilon^0 \) of the eigenstrain given by equation (4.42), we arrive at

\[
\varepsilon = \left[ I - \phi S (A + S)^{-1} \right] : \varepsilon^0 + \phi S (A + S)^{-1} (A + I) : \varepsilon^T
\]  

(4.91)

The volume-averaged stress tensor for the particles is defined as

\[
\bar{\sigma}_i = \frac{1}{V_i} \int \sigma_i (x) \, dV = \frac{1}{V_i} \int \left[ C_i : \left[ \varepsilon^0 + \varepsilon' (x) - \varepsilon^T (x) \right] \right] \, dV = C_i : \left[ \varepsilon^0 + \varepsilon' - \varepsilon^T \right]
\]  

(4.92)

where \( \varepsilon' \) can be recast as

\[
\varepsilon' = S : \left[ \frac{1}{V_i} \int \left[ \varepsilon^T (x') + \varepsilon^0 \right] \, dV' \right] = S : \left( \varepsilon_i^T + \varepsilon_i^0 \right)
\]  

(4.93)

So, we have

\[
\bar{\sigma}_i = C_i A (A + S)^{-1} : \varepsilon^0 - C_i A (I - S)(A + S)^{-1} : \varepsilon^T
\]  

(4.94)

As results of equation (4.91), the averaged internal stresses of particles can be expressed as:

\[
\bar{\sigma}_i = C_i A (A + S)^{-1} \left[ I - \phi S (A + S)^{-1} \right] : \varepsilon
\]

\[
- C_i A (A + S)^{-1} \left\{ \phi S (A + S)^{-1} (A + I) \left[ I - \phi S (A + S)^{-1} \right] + (I - S) \right\} : \varepsilon^T
\]

(4.95)

where

\[
U = C_i A (A + S)^{-1} \left[ I - \phi S (A + S)^{-1} \right]^{-1}
\]  

(4.96)

\[
V = C_i A (A + S)^{-1} \left\{ \phi S (A + S)^{-1} (A + I) \left[ I - \phi S (A + S)^{-1} \right]^{-1} + (I - S) \right\}
\]  

(4.97)

By carrying out the lengthy algebra, the components of the positive definite fourth-rank tensor \( U \) and \( V \) are explicitly given by
\[ U_{ijkl} = U_1 \delta_{ij} \delta_{kl} + U_2 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \]  
\[ (4.98) \]

\[ V_{ijkl} = V_1 \delta_{ij} \delta_{kl} + V_2 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \]  
\[ (4.99) \]

where

\[ 3U_1 + 2U_2 = \frac{(3\alpha + 2\beta) - 10(1 + v_0)}{(3\alpha + 2\beta) - 10(1 + v_0)} \cdot 3k_1 \]  
\[ (4.100) \]

\[ U_2 = \frac{\beta - (8 - 10v_0)}{\beta - (8 - 10v_0)} \cdot \mu \]  
\[ (4.101) \]

\[ 3V_1 + 2V_2 = \frac{30(1 + v_0) k_1^2}{(k_1 - k_0)(3\alpha + 2\beta)} \left[ \frac{(3\alpha + 2\beta) - 10(1 + v_0)}{(3\alpha + 2\beta) - 10(1 + v_0)} \cdot \phi - 1 \right] + 3k_1 \]  
\[ (4.102) \]

\[ V_2 = \frac{(8 - 10v_0) \mu^2}{(\mu - \mu_0) \beta} \left[ \frac{\beta - (8 - 10v_0)}{\beta - (8 - 10v_0)} \cdot \phi - 1 \right] + \mu \]  
\[ (4.103) \]

4.4 Pairwise Interacting Solution for Two-Phase Composites

In this section, we extend the noninteracting solution for two-phase composites developed in section 4.3 to account for the inter-particle interactions.

4.4.1 Approximate Solution of Two-Phase Interaction

If we neglect the inter-particle interaction effects, then the ensemble-volume averaged perturbed strain \( \bar{\varepsilon}^o \) can be dropped. The resulting noninteracting approximation for the particles becomes

\[ -A : \bar{\varepsilon}^o = \varepsilon^0 - \varepsilon^T + S : \varepsilon^T + S : \bar{\varepsilon}^o \]  
\[ (4.104) \]
Within the present two-sphere context, the integral equation governing the distributed
eigenstrain \( \varepsilon^* \) for a given particle configuration and remote strain field \( \varepsilon^0 \) can be
rephrased as

\[
-A : \varepsilon^{*(i)} (x) = \varepsilon^0 - \varepsilon^T (x) + \int_{\Omega_j} G(x - x') \left[ \varepsilon^T (x') + \varepsilon^{*(j)} (x') \right] d'x' \\
+ \int_{\Omega_j} G(x - x') \left[ \varepsilon^T (x') + \varepsilon^0 (x') \right] d'x' \quad (i \neq j, \quad i, j = 1, 2)
\]

(4.105)

where assuming \( \varepsilon^T \) is uniform in the particles.

By subtracting the noninteracting solution equation (4.104), the effect of the inter-
particles interaction can be founded by solving the following integral equation

\[
-A : d^{*(i)} (x) = \int_{\Omega_j} G(x - x') : d^{*(j)} (x') d'x' + \int_{\Omega_j} G(x - x') : \varepsilon^0 (x') d'x' \\
+ \int_{\Omega_j} G(x - x') : \left[ \varepsilon^T (x') + \varepsilon^0 \right] d'x' \quad (i \neq j, \quad i, j = 1, 2)
\]

(4.106)

where \( d^{*(i)} \) is given by

\[
d^{*(i)} = \varepsilon^{*(i)} - \varepsilon^0 \quad (4.107)
\]

Following the procedure described in Ju and Chen (1994b), the approximate equations
for \( \overline{d}^{*(i)} \) for the two-sphere interaction problem can be obtained:

\[
-A : \overline{d}^{*(i)} = S : \overline{d}^{*(i)} + G^1 (x_i - x_j) : \overline{d}^{*(j)} + G^2 (x_i - x_j) : \left( \varepsilon^T + \varepsilon^0 \right) + 0 \left( \rho^8 \right)
\]

(4.108)

where

\[
G^1 (x_i - x_j) = \frac{\rho^3}{30(1 - \nu_o)} (H^i + \rho^8 H^i)
\]

(4.109)

\[
G^2 (x_i - x_j) = \frac{\rho^3}{30(1 - \nu_o)} (H^i + 2 \rho^8 H^i)
\]

(4.110)

and \( 0 (\rho^8) \) denotes the terms which are higher than the order of \( \rho^6 \).
Where $r = \mathbf{x}_i - \mathbf{x}_j$, $r = | \mathbf{r} |$, $\rho = a/r$ and $a$ is the radius of a spherical particle. The components of $\mathbf{H}^1$ and $\mathbf{H}^2$ are given by equations (4.40) and (4.41).

Furthermore, we observe that

$$d^\alpha = d^\nu = \bar{d}$$

Therefore, the solution of equation (4.107) is given by

$$\bar{d}^\alpha = -30(1-v_0)T^{-1} \cdot G^2 : \left( \sigma^T + \sigma^0 \right) + 0(\rho^8)$$

where

$$T(x_i - x_j) = 30(1-v_0)[A + S + G^2(x_i - x_j)]$$

The procedure for finding the inverse of the fourth-rank tensor $T$ is given in the Appendix. The corresponding expression to the order of $0(\rho^3)$ is

$$T^{-1} = K^{-1} + \rho^3L + \cdots$$

where

$$K_{ijkl} = F_{ijkl} (0,0,0,0,\alpha,\beta)$$

and

$$L_{ijkl} = \frac{5}{4\beta^2} F_{ijkl} \left( -15,3v_0, \frac{6\alpha(1-2v_0)}{3\alpha + 2\beta}, \frac{6\alpha(1+v_0)}{3\alpha + 2\beta}, -\frac{2\alpha(2-v_0)}{3\alpha + 2\beta}, 1-2v_0 \right)$$

with $\alpha$ and $\beta$ given in equations (4.5) and (4.6).

The final expression for $\bar{d}$ is:

$$\bar{d}^\alpha = -\rho^3 \left[ K^{-1} \cdot \left( \mathbf{H}^1 + 2\rho^2\mathbf{H}^2 \right) \right] : \left( \sigma^T + \sigma^0 \right) - \rho^5 \left( L \cdot \mathbf{H}^1 \right) : \left( \sigma^T + \sigma^0 \right) + 0(\rho^8)$$

To obtain the ensemble-average solution of $\bar{d}^\alpha$ within the context of approximate pairwise particle interaction, one has to integrate equation (4.117) over all possible
positions $\mathbf{x}_2$ of the second particle for a given location of the first particle $\mathbf{x}_1$. The ensemble-average process can be expressed as

$$\langle \mathbf{d}^* \rangle = \int_{\nu\cdot\Omega} \mathbf{d}^* (\mathbf{x}_1 - \mathbf{x}_2) P(\mathbf{x}_2 | \mathbf{x}_1) d\mathbf{x}_2 \quad (4.118)$$

In the absence of actual manufacturing and microstructural evidences, it is often assumed that the two-point conditional probability function is statically isotropic, uniform and obeys the following form:

$$P(\mathbf{x}_2 | \mathbf{x}_1) = \begin{cases} \frac{N}{V} & \text{if } |\mathbf{x}_2 - \mathbf{x}_1| \geq 2a \\ 0 & \text{otherwise} \end{cases} \quad (4.119)$$

where $N/V$ is the number density of particles in a composite. Accordingly, the ensemble integration of equation (4.118) can be rephrased as:

$$\langle \mathbf{d}^* \rangle = -\frac{N}{V} \left[ \mathbf{K}^{-1} \cdot \left[ \int_{\frac{2a}{\sigma}}^\infty \rho^3 \int_{\mathcal{A}} \mathbf{H}^T dA d\rho + 2 \int_{\frac{2a}{\sigma}}^\infty \rho^5 \int_{\mathcal{A}} \mathbf{H}^2 dA d\rho \right] : \left( \mathbf{\varepsilon}^T + \mathbf{\varepsilon}^q \right) \right]$$

$$-\frac{N}{V} \left[ \int_{\frac{2a}{\sigma}}^\infty \rho^6 \int_{\mathcal{A}} \left( \mathbf{L} \cdot \mathbf{H}^T \right) dA d\rho \right] : \left( \mathbf{\varepsilon}^T + \mathbf{\varepsilon}^q \right) + \mathbf{0} \left( \rho^8 \right) \quad (4.120)$$

where $\mathcal{A}$ denotes the spherical surface with radius $r$. After lengthy but straightforward mathematical manipulation, the final expression takes the form:

$$\langle \mathbf{\varepsilon}^* \rangle = \mathbf{\Gamma} : \mathbf{\varepsilon}^q + \mathbf{\Gamma}^* : \mathbf{\varepsilon}^T \quad (4.121)$$

The components of the positive definite fourth-rank tensor $\mathbf{\Gamma}$ and $\mathbf{\Gamma}^*$ read

$$\Gamma_{ijkl} = \gamma_1 \delta_i^k \delta_j^l + \gamma_2 \left( \delta_i^k \delta_j^l + \delta_i^l \delta_j^k \right) \quad (4.122)$$

$$\Gamma^*_{ijkl} = \gamma_1 \delta_i^k \delta_j^l + \gamma^* \left( \delta_i^k \delta_j^l + \delta_i^l \delta_j^k \right) \quad (4.123)$$

Where
\[
\gamma_i^* = \frac{5\phi}{8\beta^2} \left\{ (13 - 14v_o)\nu_o - \frac{8\alpha}{3\alpha + 2\beta} (1 - 2v_o)(1 + \nu_o) \right\} \\
(4.124)
\]

\[
\gamma_2^* = \frac{5\phi}{16\beta^2} \left\{ (25 - 34v_o + 22v_o^2) - \frac{6\alpha}{3\alpha + 2\beta} (1 - 2v_o)(1 + \nu_o) \right\} \\
(4.125)
\]

with \(\gamma_i\) and \(\gamma_2\) are given in equations (4.7) and (4.8).

### 4.4.2 Average Stress Norm in Matrix

Following Ju and Chen (1994a), the total stress at any point \(\mathbf{x}\) in the matrix is given by the superposition of the far-field stress \(\sigma_0\) and the perturbed stress \(\sigma'\) induced by the particles. Assuming the elastic eigenstrain in the particle \(\varepsilon^*\) is uniform, the perturbed stress for any matrix point \(\mathbf{x}\) takes the form

\[
\sigma'(\mathbf{x}|\mathbf{x}_i) = \left[ C_0 \cdot \mathbf{G}(\mathbf{x} - \mathbf{x}_i) \right] : (\varepsilon^* + \varepsilon^0) \\
(4.126)
\]

Where \(\varepsilon^0\) is the eigenstrain caused by the CTE mismatch between the matrix and the particle. Using the ensemble-volume averaged eigenstrain given in equation (4.121), the stress perturbation can be rephrased as:

\[
\sigma'(\mathbf{x}|\mathbf{x}_i) = \left[ C_0 \cdot \mathbf{G}(\mathbf{x} - \mathbf{x}_i) \cdot \Gamma \right] : (\varepsilon^* + \varepsilon^0) \\
(4.127)
\]

where \(\varepsilon^0\) denotes the solution of the eigenstrain for the single inclusion problem, which is given by equation (4.42). Therefore,

\[
\sigma'(\mathbf{x}|\mathbf{x}_i) = -\left[ C_0 \cdot \mathbf{G} \cdot \Gamma (A + S)^{-1} \right] : \varepsilon^0 + \left[ C_0 \cdot \mathbf{G} \cdot \Gamma (A + S)^{-1}(A + I) \right] : \varepsilon^0 \\
(4.128)
\]

Following the same procedure used for the noninteracting solution, we obtain the ensemble-averaged current stress norm at any matrix point \(\mathbf{x}\) as:

\[
\langle H \rangle_m (\mathbf{x}) = \sigma^0 : \mathbf{T} : \sigma^0 + \sigma^* : \mathbf{T} : \sigma^* - 2\sigma^0 : \mathbf{T} : \sigma^* \\
(4.129)
\]
where $\sigma^T$ is given by equation (4.56), and the components of the positive definite fourth-rank tensor $T$ and $T^*$ read:

$$T_{ijkl} = T^*_{ijkl} \delta_{ij} \delta_{kl} + T^*_2 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right)$$  \hspace{1cm} (4.130)

$$T^*_{ijkl} = T^*_{ijkl} \delta_{ij} \delta_{kl} + T^*_2 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right)$$  \hspace{1cm} (4.131)

with

$$3T^*_1 + 2T^*_2 = 200(1 - 2\nu_0)^2 \frac{(3 \gamma_1 + 2 \gamma_2)^2}{(3 \alpha + 2 \beta)^2} \phi$$  \hspace{1cm} (4.132)

$$T^*_2 = \frac{1}{2} + (23 - 50\nu_0 + 35\nu_0^2) \frac{4\gamma_2^2}{\beta^2} \phi$$  \hspace{1cm} (4.133)

$$3T^*_1 + 2T^*_2 = 200(1 - 2\nu_0)^2 \frac{(3 \gamma_1 + 2 \gamma_2)^2}{(3 \alpha + 2 \beta)^2} \phi$$  \hspace{1cm} (4.134)

$$T^*_2 = (23 - 50\nu_0 + 35\nu_0^2) \frac{4\gamma_2^2}{\beta^2} \phi$$  \hspace{1cm} (4.135)

$\alpha$ and $\beta$ are given in equations (4.5) and (4.6).

The ensemble-averaged current stress norm at a matrix point can also be expressed in terms of the macroscopic stress $\bar{\sigma}$. Following the same procedure as in former section, the relation between the far-field stress $\sigma^f$ and the macroscopic stress $\bar{\sigma}$ takes the form:

$$\bar{\sigma} = P : \sigma^f - Q : \sigma^T$$  \hspace{1cm} (4.136)

where

$$P = I + \phi (I - S) \Gamma (A + S)^{-1}$$  \hspace{1cm} (4.137)

$$Q = \phi (I - S) \Gamma (A + S)^{-1}$$  \hspace{1cm} (4.138)

where the components of $P$ and $Q$ are given:
\[ P_{ijkl} = P_1 \delta_{ij} \delta_{kl} + P_2 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \]  
(4.139)

\[ Q_{ijkl} = Q_1 \delta_{ij} \delta_{kl} + Q_2 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \]  
(4.140)

with

\[ 3P_1 + 2P_2 = a\phi + 1 \]  
(4.141)

\[ P_2 = \frac{1}{2} \left( b\phi + 1 \right) \]  
(4.142)

\[ 3Q_1 + 2Q_2 = a\phi \]  
(4.143)

\[ Q_2 = \frac{1}{2} b\phi \]  
(4.144)

\[ a = 20(1 - 2\nu) \frac{3\gamma_1 + 2\gamma_2}{3\alpha + 2\beta} \]  
(4.145)

\[ b = (7 - 5\nu) \frac{2\gamma_2}{\beta} \]  
(4.146)

Using equation (4.136), we arrive at the alternative expression for the ensemble-averaged current stress norm in a matrix point \( x \):

\[ \langle H \rangle \_w (x) = \overline{\sigma} : \overline{T} : \overline{\sigma} + 2\overline{\sigma} : \overline{T} : \overline{\sigma}^T + \overline{\sigma}^T : \overline{\sigma}^T \]  
(4.147)

where the positive definite fourth-rank tensor \( \overline{T} \), \( \overline{T}^\prime \), and \( \overline{T}^{\prime\prime} \) are defined as

\[ \overline{T} = \left( P^{-1} \right)^T \cdot T \cdot P^{-1} \]  
(4.148)

\[ \overline{T}^\prime = \left( P^{-1} \right)^T \cdot T \cdot P^{-1} \cdot Q - T^\prime \cdot P^{-1} \]  
(4.149)

\[ \overline{T}^{\prime\prime} = \left( P^{-1} \cdot Q \right)^T \cdot T \cdot \left( P^{-1} \cdot Q \right) + T^\prime - 2T^\prime \cdot \left( P^{-1} \cdot Q \right) \]  
(4.150)

where the components of \( \overline{T} \), \( \overline{T}^\prime \), and \( \overline{T}^{\prime\prime} \) are

\[ \overline{T}_{ijkl} = \overline{T_1} \delta_{ij} \delta_{kl} + \overline{T_2} \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \]  
(4.151)
\[
\begin{aligned}
\bar{T}_{ijkl}^* &= \bar{T}_1 \delta_{ij} \delta_{kl} + \bar{T}_2 (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \\
\bar{T}_{ijkl}^{**} &= \bar{T}_1 \delta_{ij} \delta_{kl} + \bar{T}_2 (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})
\end{aligned}
\]  
(4.152)

with

\[
3 \bar{T}_1 + 2 \bar{T}_2 = \frac{3T_1 + 2T_2}{(a \phi + 1)^2}
\]  
(4.154)

\[
\bar{T}_2 = \frac{T_2}{(b \phi + 1)^2}
\]  
(4.155)

\[
3 \bar{T}_1^* + 2 \bar{T}_2^* = -\frac{3T_1 + 2T_2}{(a \phi + 1)^2}
\]  
(4.156)

\[
\bar{T}_2^* = -\frac{T_2}{(b \phi + 1)^2} + \frac{1}{2(b \phi + 1)}
\]  
(4.157)

\[
3 \bar{T}_1^{**} + 2 \bar{T}_2^{**} = \frac{3T_1 + 2T_2}{(a \phi + 1)^2}
\]  
(4.158)

\[
\bar{T}_2^{**} = \frac{T_2}{(b \phi + 1)^2} + \frac{b \phi - 1}{2(b \phi + 1)}
\]  
(4.159)

Because \( \sigma^T = AC_1 : \epsilon^T \) caused by CTE mismatch is spherical stress, equation (4.147) of the ensemble-averaged loading function can be simplified as

\[
\langle H \rangle_m (x) = \left( \bar{\sigma} - \bar{\sigma}^r \right) : \bar{T} : \left( \bar{\sigma} - \bar{\sigma}^r \right)
\]  
(4.160)

### 4.4.3 Average Stress in Particles

The ensemble-volume averaged strain for two-phase composites takes the form

\[
\bar{\epsilon} = \bar{\epsilon}^0 + \phi S : \left( \bar{\epsilon}^T + \bar{\epsilon}^* \right)
\]  
(4.161)

As results of equation (4.121), we have
\[ \bar{\varepsilon} = \varepsilon^0 + \phi \Sigma : \left( \bar{\varepsilon}^T + \bar{\varepsilon}^0 \right) \]  

(4.162)

With the noninteracting solution \( \bar{\varepsilon}^0 \) of the eigenstrain given by equation (4.42), we arrive at:

\[ \bar{\varepsilon} = \left[ I - \phi \Sigma \left( A + S \right)^{-1} \right] : \varepsilon^0 + \phi \left[ \Sigma \left( A + S \right)^{-1} \left( A + I \right) \right] : \bar{\varepsilon}^T \]  

(4.163)

The volume-averaged stress tensor for the particles is defined as:

\[ \bar{\sigma}_i = \frac{1}{V_i} \int_{V_i} \sigma_i (x) dV = \frac{1}{V_i} \int_{V_i} C_i : \left[ \varepsilon^0 + \varepsilon'(x) - \varepsilon^T (x) \right] dx = C_i : \left[ \varepsilon^0 + \bar{\varepsilon}' - \bar{\varepsilon}^T \right] \]  

(4.164)

where \( \bar{\varepsilon}' \) can be recast as

\[ \bar{\varepsilon}' = S : \left( \frac{1}{V_i} \int_{V_i} \left[ \varepsilon'(x) + \varepsilon'(x') \right] dV \right) = S \Sigma : \left( \bar{\varepsilon}^T + \bar{\varepsilon}^0 \right) \]  

(4.165)

Using equation (4.165), we have

\[ \bar{\sigma}_i = C_i : \varepsilon^0 + \left[ C_i (S \Sigma - I) \right] : \bar{\varepsilon}^T + \left[ C_i S \Sigma \right] : \varepsilon^0 \]  

(4.166)

With the noninteracting solution \( \bar{\varepsilon}^0 \) of the eigenstrain, we arrive at

\[ \bar{\sigma}_i = C_i \left[ I - S \Sigma \left( A + S \right)^{-1} \right] : \varepsilon^0 + C_i \left[ S \Sigma \left( A + S \right)^{-1} \left( A + I \right) - I \right] : \bar{\varepsilon}^T \]  

(4.167)

Combing with equation (4.163), the averaged internal stresses of particles can be expressed as:

\[ \bar{\sigma}_i = C_i \left[ I - S \Sigma \left( A + S \right)^{-1} \right] \left[ I - \phi \Sigma \left( A + S \right)^{-1} \right] : \bar{\varepsilon} - C_i \left[ \phi \Sigma \left( I - S \Sigma \left( A + S \right)^{-1} \right) \right] \left[ I - \phi \Sigma \left( A + S \right)^{-1} \right]^{-1} \left( A + S \right)^{-1} \left( A + I \right) - \left[ S \Sigma \left( A + S \right)^{-1} \left( A + I \right) - I \right] : \bar{\varepsilon}^T \]  

(4.168)

\[ = U : \bar{\varepsilon} - V : \bar{\varepsilon}^T \]

where

\[ U = C_i \left[ I - S \Sigma \left( A + S \right)^{-1} \right] \left[ I - \phi \Sigma \left( A + S \right)^{-1} \right] \]  

(4.169)
\[
V = C_1 \phi \Sigma \left[ \mathbf{I} - \mathbf{S} \Gamma (\mathbf{A} + \mathbf{S})^{-1} \right] \left[ \mathbf{I} - \phi \mathbf{S} \Gamma (\mathbf{A} + \mathbf{S})^{-1} \right]^{-1} (\mathbf{A} + \mathbf{S})^{-1} (\mathbf{A} + \mathbf{l})
\]

\[
- \left[ \mathbf{S} \Gamma (\mathbf{A} + \mathbf{S})^{-1} (\mathbf{A} + \mathbf{l})^{-1} \right] \}
\]

(4.170)

By carrying out the lengthy algebra, the components of the positive definite fourth-rank tensor \( \mathbf{U} \) and \( \mathbf{V} \) are explicitly given by:

\[
U_{ijkl} = U_1 \delta_{ij} \delta_{kl} + U_2 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right)
\]

(4.171)

\[
V_{ijkl} = V_1 \delta_{ij} \delta_{kl} + V_2 \left( \delta_{il} \delta_{jk} + \delta_{ij} \delta_{kl} \right)
\]

(4.172)

where

\[
3U_1 + 2U_2 = \frac{(3\alpha + 2\beta) - 10(1 + \nu_0)(3\gamma_1 + 2\gamma_2)}{(3\alpha + 2\beta) - 10(1 + \nu_0)\phi(3\gamma_1 + 2\gamma_2)} \cdot 3k_i
\]

(4.173)

\[
U_2 = \frac{\beta - 4(4 - 5\nu_0)\gamma_2}{\beta - 4(4 - 5\nu_0)\phi \gamma_2} \cdot \mu_i
\]

(4.174)

\[
3V_1 + 2V_2 = \frac{30(1 + \nu_0)(3\gamma_1 + 2\gamma_2)k_i^2}{(k_i - k_0)(3\alpha + 2\beta)} \left[ \frac{(3\alpha + 2\beta) - 10(1 + \nu_0)(3\gamma_1 + 2\gamma_2)}{(3\alpha + 2\beta) - 10(1 + \nu_0)\phi(3\gamma_1 + 2\gamma_2)} \cdot \phi - 1 \right] + 3k_i
\]

(4.175)

\[
V_2 = \frac{4(4 - 5\nu_0)\gamma_2 \mu_i}{(\mu_i - \mu_0)\beta} \left[ \frac{\beta - 4(4 - 5\nu_0)\gamma_2}{\beta - 4(4 - 5\nu_0)\gamma_2 \phi} \cdot \phi - 1 \right] + \mu_i
\]

(4.176)

### 4.5 Noninteracting Solution for Three-Phase Composites

Let us consider an initially perfectly bonded two-phase composite consisting of an elastic matrix (phase 0) with bulk modulus \( k_0 \) and shear modulus \( \mu_0 \), and randomly dispersed elastic spherical particles (phase 1) with bulk modulus \( k_1 \) and shear modulus \( \mu_1 \). Subsequently, as loadings or deformations are applied, some particles could...
experience complete interfacial debonding. These completely debonded particles can be regarded as spherical voids (phase 2).

### 4.5.1 Effective Elastic Modulus of Multiphase Composites

Effective elastic moduli of multi-phase composites containing randomly located, unidirectionally aligned elastic ellipsoids were explicitly derived by Ju and Chen (1994a).

For a multi-phase composite, the effective (noninteracting) elasticity tensor $\mathbf{C}$, reads

$$\mathbf{C}_e = \mathbf{C}_0 \cdot \left[ \mathbf{I} + \mathbf{B} \cdot (\mathbf{I} - \mathbf{S} \cdot \mathbf{B})^{-1} \right]$$

(4.177)

where $\mathbf{B}$ takes the form

$$\mathbf{B} = \sum_{q=1}^{s} \phi_q \left( \mathbf{S} + \mathbf{A}_q \right)^{-1}$$

(4.178)

Since the phase 2 contains spherical voids, we have $\mathbf{A}_2 = -\mathbf{I}$. The effective bulk modulus $k_*$ and shear modulus $\mu_*$ for the three-phase composite ($n=2$) can be explicitly expressed as

$$k_* = k_0 \left\{ 1 + \frac{30(1-v_0)\sum_{q=1}^{2} \frac{\phi_q}{3\alpha_q + 2\beta_q}}{1-10(1+v_0)\sum_{q=1}^{2} \frac{\phi_q}{3\alpha_q + 2\beta_q}} \right\}$$

(4.179)

$$\mu_* = \mu_0 \left\{ 1 + \frac{15(1-v_0)\sum_{q=1}^{2} \frac{\phi_q}{\beta_q}}{1-2(4-5v_0)\sum_{q=1}^{2} \frac{\phi_q}{\beta_q}} \right\}$$

(4.180)

with

$$\alpha_q = 2(5v_0 - 1) + 10(1-v_0) \left( \frac{k_0}{k_q - k_0} - \frac{\mu_0}{\mu_q - \mu_0} \right)$$

(4.181)
\[
\beta_q = 2(4 - 5v_0) + 15(1 - v_0) \frac{\mu_0}{\mu_q - \mu_0} \tag{4.182}
\]

### 4.5.2 Average Stress Norm in Matrix

According to the Eshelby theory, the perturbed stress \( \sigma' \) at any point in the matrix due to the presence of the particles and voids can be written as:

\[
\sigma'(x) = C_q : \left[ \int_{V} G(x - x') : (\varepsilon_x^r + \varepsilon_z^r) \, dx' + C_q : \left[ \int_{V} G(x - x') : (\varepsilon_x^r + \varepsilon_z^r) \, dx' \right] \right]
\]

The eigenstrain in a single ellipsoidal inclusion is uniform for the interior points of an isolated (noninteracting) inclusion. Therefore, the perturbed stress for any matrix point \( x \) due to a typical isolated \( \varphi \)-phase inhomogeneity centered at \( x_q \) takes the form

\[
\sigma'(x|x_q) = [C_\varphi \cdot \bar{G}(x - x_q)] : (\varepsilon_x^{\varphi} + \varepsilon_z^{\varphi})
\]

where \( \bar{G}(x - x_q) \) is given by equation (4.39), and

\[
\varepsilon_x^{\varphi} = -\left((A_q + S)^{-1}\right) : \varepsilon^p + \left((A_q + S)^{-1}(I - S)\right) : \varepsilon^{\varphi}
\]

We denote by \( H(x|\varphi) \) the square of the current stress norm at the local point \( x \), which determines the plastic strain for a given phase configuration \( \varphi \). Since there is no plastic strain in the elastic particles or voids, \( H(x|\varphi) \) can be written as

\[
H(x|\varphi) = \begin{cases} \sigma(x|\varphi) : I : \sigma(x|\varphi) & \text{if } x \text{ in matrix} \\ 0 & \text{otherwise} \end{cases}
\]

In addition, \( \langle H \rangle_m(x) \) is defined as the ensemble average of \( H(x|\varphi) \) over all possible realizations where \( x \) is in the matrix phase. Matrix point receives perturbations from particles and voids. Therefore, the ensemble-average stress norm for any matrix point \( x \)
can be evaluated by collecting and summing up all the current stress norm perturbations produced by any typical particle centered at $\mathbf{x}_i$ in the particle domain and any typical void centered at $\mathbf{x}_2$ in the void domain, and averaging over all possible locations of $\mathbf{x}_i$ and $\mathbf{x}_2$.

$$
\langle H \rangle_m (\mathbf{x}) = H^0 + \int_{\eta > a} \left\{ H \left( \mathbf{x} | \mathbf{x}_i \right) - H^0 \right\} P (\mathbf{x}_i) \, d\mathbf{x}_i + \int_{\eta > a} \left\{ H \left( \mathbf{x} | \mathbf{x}_2 \right) - H^0 \right\} P (\mathbf{x}_2) \, d\mathbf{x}_2 \quad (4.187)
$$

where $r_i = |\mathbf{x} - \mathbf{x}_i|$, $r_2 = |\mathbf{x} - \mathbf{x}_2|$, $P(\mathbf{x}_i)$ and $P(\mathbf{x}_2)$ denote the probability density functions for finding a particle centered at $\mathbf{x}_i$ and a void centered at $\mathbf{x}_2$, respectively. For simplicity, $P(\mathbf{x}_i)$ and $P(\mathbf{x}_2)$ are assumed to be statistically homogeneous, isotropic and uniform. Using the properties of the fourth-order tensor $\mathbf{G}(\mathbf{x} - \mathbf{x}_q)$, we obtain the ensemble-averaged current stress norm at any matrix point $\mathbf{x}$ as:

$$
\langle H \rangle_m (\mathbf{x}) = H^0 + \frac{N_1}{V} \int_{\eta > a} dr_i \int_{\lambda(\eta)} \left( \sigma^i \left( \mathbf{x} | \mathbf{x}_i \right) : \mathbf{I}_d : \sigma^i \left( \mathbf{x} | \mathbf{x}_i \right) \right) d\mathbf{A} \\
+ \frac{N_2}{V} \int_{\eta > a} dr_2 \int_{\lambda(\eta)} \left( \sigma^2 \left( \mathbf{x} | \mathbf{x}_2 \right) : \mathbf{I}_d : \sigma^2 \left( \mathbf{x} | \mathbf{x}_2 \right) \right) d\mathbf{A} 
$$

(4.188)

By carrying out the lengthy but straightforward algebra, we have

$$
\langle H \rangle_m (\mathbf{x}) = \sigma^0 : \mathbf{T} : \sigma^0 + \sigma^T : \mathbf{T}^\top : \sigma^T - 2\sigma^0 : \mathbf{T} : \sigma^T
$$

(4.189)

where

$$
\sigma^T = \Lambda \mathbf{C} : \mathbf{e}^T
$$

(4.190)

The components of the positive definite fourth-rank tensor $\mathbf{T}$ and $\mathbf{T}^\top$ read

$$
T_{ijkl} = T_{ij} \delta_{ij} \delta_{kl} + T_2 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right)
$$

(4.191)

$$
T_{ijkl}^* = T_{ij}^* \delta_{ij} \delta_{kl} + T_2^* \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right)
$$

(4.192)

with
The ensemble-averaged current stress norm at a matrix point must be established in terms of the macroscopic stress $\bar{\sigma}$ in order to express the effective loading function in terms of the macroscopic stress. In the special case of uniform dispersions of identical elastic spheres in a homogeneous matrix, the macroscopic stress and the far-field stress take the form:

$$\bar{\sigma} = C_0 \left[ \bar{\epsilon} - \sum_{q=1}^{2} \phi_q \left( \bar{\epsilon}_q^0 + \bar{\epsilon}_q^r \right) \right]$$

$$\sigma^0 = C_0 \left[ \bar{\epsilon} - \sum_{q=1}^{2} \phi_q S \left( \bar{\epsilon}_q^0 + \bar{\epsilon}_q^r \right) \right]$$

Using equations (4.197), (4.198) & (4.185), the relation between the far-field stress $\sigma^0$ and the macroscopic stress $\bar{\sigma}$ takes the form

$$\bar{\sigma} = P : \sigma^0 - Q : \sigma^r$$

where

$$P = I + \sum_{q=1}^{2} \phi_q \left( I - S \right) \left( A_q + S \right)^{-1}$$

$$Q = \phi_1 \left( I - S \right) \left( A_1 + S \right)^{-1}$$
with the components of $P$ and $Q$ are

\[
P_{ijkl} = P_1\delta_{ij}\delta_{kl} + P_2\left(\delta_{ik}\delta_{jl} + \delta_{ij}\delta_{lk}\right) \tag{4.202}
\]

\[
Q_{ijkl} = Q_1\delta_{ij}\delta_{kl} + Q_2\left(\delta_{ik}\delta_{jl} + \delta_{ij}\delta_{lk}\right) \tag{4.203}
\]

where

\[
3P_1 + 2P_2 = \sum_{q=1}^{2} a_q \phi_q + 1 \tag{4.204}
\]

\[
P_2 = \frac{1}{2}\left(\sum_{q=1}^{2} b_q \phi_q + 1\right) \tag{4.205}
\]

\[
3Q_1 + 2Q_2 = a_1 \phi_1 \tag{4.206}
\]

\[
Q_2 = \frac{1}{2} b_1 \phi_1 \tag{4.207}
\]

\[
a_q = \frac{20(1-2\nu_q)}{3\alpha_q + 2\beta_q} \tag{4.208}
\]

\[
b_q = \frac{(7-5\nu_q)}{\beta_q} \tag{4.209}
\]

Using equations (4.199) and (4.189), we arrive at the alternative expression for the ensemble-averaged current stress norm in a matrix point $x$ as:

\[
\langle H \rangle_w (x) = \bar{\sigma} : \bar{T} : \bar{\sigma} + 2\bar{\sigma} : \bar{T} : \bar{\sigma} + \bar{\sigma} : \bar{T} : \bar{\sigma} \tag{4.210}
\]

where the positive definite fourth-rank tensor $\bar{T}$, $\bar{T}$, and $\bar{T}$ are defined as

\[
\bar{T} = (P^{-1})^T \cdot T \cdot P^{-1} \tag{4.211}
\]

\[
\bar{T} = (P^{-1})^T \cdot T \cdot P^{-1} \cdot Q - T \cdot P^{-1} \tag{4.212}
\]

\[
\bar{T} = (P^{-1} \cdot Q)^T \cdot T \cdot (P^{-1} \cdot Q) + T - 2T \cdot (P^{-1} \cdot Q) \tag{4.213}
\]

where the components of $\bar{T}$, $\bar{T}$, and $\bar{T}$ are
\[ \bar{T}_{ijkl} = T_1 \delta_{ij} \delta_{kl} + T_2 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \]  
(4.214)

\[ \bar{T}^*_{ijkl} = T_1^* \delta_{ij} \delta_{kl} + T_2^* \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \]  
(4.215)

\[ \bar{T}^{**}_{ijkl} = T_1^{**} \delta_{ij} \delta_{kl} + T_2^{**} \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \]  
(4.216)

with

\[ 3\bar{T}_1 + 2\bar{T}_2 = \frac{3T_1 + 2T_2}{\left( \sum_{q=1}^{2} a_q \phi_q + 1 \right)^2} \]  
(4.217)

\[ \bar{T}_2 = \frac{\frac{T_2}{2}}{\left( \sum_{q=1}^{2} b_q \phi_q + 1 \right)^2} \]  
(4.218)

\[ 3\bar{T}_1^* + 2\bar{T}_2^* = -\frac{3T_1^* + 2T_2^*}{\left( \sum_{q=1}^{2} a_q \phi_q + 1 \right)^2} \]  
(4.219)

\[ \bar{T}_2^* = -\frac{T_2}{\left( \sum_{q=1}^{2} b_q \phi_q + 1 \right)^2} + \frac{1}{2 \left( \sum_{q=1}^{2} b_q \phi_q + 1 \right)} \]  
(4.220)

\[ 3\bar{T}_1^{**} + 2\bar{T}_2^{**} = \frac{3T_1^{**} + 2T_2^{**}}{\left( \sum_{q=1}^{2} a_q \phi_q + 1 \right)^2} \]  
(2.221)

\[ \bar{T}_2^{**} = \frac{T_2}{\left( \sum_{q=1}^{2} b_q \phi_q + 1 \right)^2} + \frac{\sum_{q=1}^{2} b_q \phi_q - 1}{2 \left( \sum_{q=1}^{2} b_q \phi_q + 1 \right)} \]  
(4.222)

Because \( \sigma^T = AC_t : \varepsilon^T \) caused by the CTE mismatch is spherical stress, so equation (4.147) of the ensemble-averaged loading function can be simplified as:

\[ \langle H \rangle = (\bar{\sigma} - \bar{\sigma}^*) : \bar{T} : (\bar{\sigma} - \bar{\sigma}^*) \]  
(4.223)
4.5.3 Average Stress in Particles

The ensemble-volume averaged strain for three-phase composites takes the form

\[ \overline{\varepsilon} = \varepsilon^0 + \sum_{q=1}^{2} \phi_q S \left( \overline{\varepsilon}_q^{*0} + \overline{\varepsilon}_q^T \right) \]  (4.224)

With the noninteracting solution \( \overline{\varepsilon}^{*0} \) of the eigenstrain given by equation (4.185), we arrive at

\[ \overline{\varepsilon} = \left[ I - \sum_{q=1}^{2} \phi_q S (A_q + S)^{-1} \right]: \varepsilon^0 + \phi_1 S (A_1 + S)^{-1} (A_1 + I): \overline{\varepsilon}_1^T \]  (4.225)

The volume-averaged stress tensor for the particles is defined as

\[ \overline{\sigma}_i = \frac{1}{V_i} \left[ \sigma_i (x) dx \right] = \frac{1}{V_i} \left[ \int C_i : \left[ \varepsilon^0 + \varepsilon^\prime (x) - \overline{\varepsilon}^\prime (x) \right] dx - \int C_i : \left[ \varepsilon^0 + \overline{\varepsilon}^\prime - \overline{\varepsilon}^\prime_0 \right] \right] \]  (4.226)

where \( \overline{\varepsilon}^\prime_0 \) can be recast as

\[ \overline{\varepsilon}^\prime_0 = S : \left\{ \frac{1}{V_i} \int \left[ \varepsilon^\prime (x') + \varepsilon^\prime_0 \right] dx' \right\} = S : \left( \overline{\varepsilon}_i^T + \overline{\varepsilon}_i^{*0} \right) \]  (4.227)

With the help of equations (4.227) and (4.185), equation (4.226) can be rephrased as

\[ \overline{\sigma}_i = C_i A_i (A_i + S)^{-1} : \varepsilon^0 - C_i A_i (I - S) (A_i + S)^{-1} : \overline{\varepsilon}_i^T \]  (4.228)

As results of equation (4.225), the average internal stress of particles can be expressed as:

\[ \overline{\sigma}_i = C_i A_i (A_i + S)^{-1} \left[ I - \sum_{q=1}^{2} \phi_q S (A_q + S)^{-1} \right]^{-1} : \overline{\varepsilon} \]

\[- C_i A_i (A_i + S)^{-1} \left\{ \phi_1 S (A_1 + S)^{-1} (A_1 + I) \left[ I - \sum_{q=1}^{2} \phi_q S (A_q + S)^{-1} \right]^{-1} (I - S) \right\} : \overline{\varepsilon}_1^T \]  (4.229)

where

\[ U = C_i A_i (A_i + S)^{-1} \left[ I - \sum_{q=1}^{2} \phi_q S (A_q + S)^{-1} \right]^{-1} \]  (4.230)
\[
V = C \mathbf{A} \big( \mathbf{A} + \mathbf{S} \big)^{-1} \left\{ \phi \mathbf{S} \big( \mathbf{A} + \mathbf{S} \big)^{-1} \big( \mathbf{A} + \mathbf{I} \big) \left[ \mathbf{I} - \sum_{q=1}^{2} \phi_q \mathbf{S} \big( \mathbf{A}_q + \mathbf{S} \big)^{-1} \right]^{-1} \right\} + (1 - \mathbf{S}) \tag{4.231}
\]

By carrying out the lengthy algebra, the components of the positive definite fourth-rank tensor \( \mathbf{U} \) and \( \mathbf{V} \) are explicitly given by:

\[
U_{ijkl} = U_1 \delta_{ij} \delta_{kl} + U_2 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \tag{4.232}
\]

\[
V_{ijkl} = V_1 \delta_{ij} \delta_{kl} + V_2 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \tag{4.233}
\]

where

\[
3U_1 + 2U_2 = \frac{(3 \alpha_i + 2 \beta_i) - 10(1 + v_0)}{(3 \alpha_i + 2 \beta_i) \left[ 1 - 10(1 + v_0) \sum \frac{\phi_q}{3 \alpha_q + 2 \beta_q} \right]} \cdot 3k_i \tag{4.234}
\]

\[
U_2 = \frac{\beta_i - 2(4 - 5v_0)}{\beta_i \left[ 1 - 2(4 - 5v_0) \sum \frac{\phi_q}{\beta_q} \right]} \cdot \mu_i \tag{4.235}
\]

\[
3V_1 + 2V_2 = \frac{(3 \alpha_i + 2 \beta_i) - 10(1 + v_0)}{(3 \alpha_i + 2 \beta_i) \left[ 1 - 10(1 + v_0) \sum \frac{\phi_q}{3 \alpha_q + 2 \beta_q} \left( k_i - k_0 \right) \right]} \cdot 3k_i \tag{4.236}
\]

\[
V_2 = \frac{\beta_i - 2(4 - 5v_0)}{\beta_i} \cdot \left[ \frac{2(4 - 5v_0) \phi \mu_i}{\beta_i \left[ 1 - 2(4 - 5v_0) \sum \frac{\phi_q}{\beta_q} \right] \left( \mu_i - \mu_0 \right) + \frac{7 - 5v_0}{15(1 - v_0)}} \right] \mu_i \tag{4.237}
\]
4.6 Effective Thermomechanical Properties of Composite Sphere Assemblage

In many particulate composites, a thin layer of some other elastic phase intervenes between a particle and the matrix. The imperfect interface bond may be due to the very compliant thin interfacial layer that is assumed to have perfect boundary conditions with the matrix and the particle. This defines a three-phase composite that includes particles, thin interphase, and the matrix as shown in figure 4.2. Once the effective mechanical and thermal properties of the inner composite sphere assemblage (CSA), which consists of the particle and interphase layer of thickness $\delta$, are found, the composite models used for perfect interface composite model can be readily applied to this case of imperfect interface conditions.

![Image](image.png)

**Figure 4.2 Three-phase composite system**

The composite spheres assemblage (CSA) model was first proposed by Kerner (1956) and Van der Poel (1958) as shown in figure 4.3. Smith (1974, 1975), Christensen and Lo (1979), and Hashin and his co-workers (1962, 1963, 1968, 1990, and 1991) eventually improved on the CSA model. The CSA assumes that the particles are spherical and, moreover, that the action on the particle is transmitted through a spherical interphase shell. The overall macro-behavior is assumed to be isotropic and is thus characterized by
two effective moduli: the bulk modulus $k$ and the shear modulus $\mu$. In this section, I summarized the theoretical solution for effective thermomechanical properties of the CSA consisting of an elastic spherical particle and an elastic interphase layer with a thickness of $\delta$. In the following formulae, $k$ represents the bulk modulus, $\mu$ represents shear modulus, $\alpha$ and represents the coefficient of thermal expansion. The subscripts $i$, $f$ and $m$ refer to the interphase, filler and matrix, respectively.

![Figure 4.3 Schematic illustration of composite spherical assemblage (CSA)](image)

### 4.6.1 Effective Bulk Modulus

The effective bulk modulus $k^*$ for the CSA as obtained by Hashin (1962) is given as:

$$k^* = k_i + \frac{\phi}{1 + \frac{3(1 - \phi)}{k_f - k_i + 3k_i + 4\mu_i}} \quad (4.238)$$

where

$$\phi = \left(\frac{r}{r + \delta}\right)^3 \quad (4.239)$$

$r$ is the radius of the filler particle

$\delta$ is the thickness of interphase
Hashin and Shtrikman’s formulae (1963) and Walpole’s formulae (1966) provide upper and lower bounds for the bulk modulus of the CSA. Equation (4.238) is same as the highest lower bound.

4.6.2 Effective Coefficient of Thermal Expansion (ECTE)

The effective coefficient of thermal expansion $\alpha^*$ for the CSA as obtained by Levin (1967) is given as:

$$\alpha^* = \alpha_i + \frac{\alpha_f - \alpha_i}{\frac{1}{k_f^*} - \frac{1}{k_i^*}}$$

(4.240)

4.6.3 Effective Shear Modulus

Based on the generalized self-consistent scheme (GSCS) model proposed by (Hashin, 1962), Christensen and Lo (1979) have given the condition for determining the effective shear modulus of CSA as follows:

$$A \left( \frac{\mu^*}{\mu_i} \right)^2 + B \left( \frac{\mu^*}{\mu_i} \right) + D = 0$$

(4.241)

where

$$A = 8 \left[ \mu_f / \mu_i - 1 \right] (4 - 5\nu_i) \eta_\ell \phi^{10/3} - 2 \left[ 63 \left( \mu_f / \mu_i - 1 \right) \eta_2 + 2 \eta_1 \eta_3 \right] \phi^{7/3}$$
$$+ 252 \left[ \mu_f / \mu_i - 1 \right] \eta_\ell \phi^{5/3} - 50 \left[ \mu_f / \mu_i - 1 \right] (7 - 12\nu_i + 8\nu_i^2) \eta_2 \phi + 4 (7 - 10\nu_i) \eta_2 \eta_3$$

(4.242)

$$B = -4 \left[ \mu_f / \mu_i - 1 \right] (1 - 5\nu_i) \eta_\ell \phi^{10/3} + 4 \left[ 63 \left( \mu_f / \mu_i - 1 \right) \eta_2 + 2 \eta_1 \eta_3 \right] \phi^{7/3}$$
$$- 504 \left[ \mu_f / \mu_i - 1 \right] \eta_\ell \phi^{5/3} + 150 \left[ \mu_f / \mu_i - 1 \right] (3 - \nu_i) \nu_i \eta_2 \phi + 3 (15\nu_i - 7) \eta_2 \eta_3$$

(4.243)

$$D = 4 \left[ \mu_f / \mu_i - 1 \right] (5\nu_i - 7) \eta_\ell \phi^{10/3} - 2 \left[ 63 \left( \mu_f / \mu_i - 1 \right) \eta_2 + 2 \eta_1 \eta_3 \right] \phi^{7/3}$$
$$+ 252 \left[ \mu_f / \mu_i - 1 \right] \eta_\ell \phi^{5/3} + 25 \left[ \mu_f / \mu_i - 1 \right] (5\nu_i - 7) \eta_2 \phi - (7 + 5\nu_i) \eta_2 \eta_3$$

(4.244)
with
\[
\eta_1 = \left[ \mu_f / \mu_i - 1 \right] (49 - 50\nu_f \nu_i) + 35 (\mu_f / \mu_i) (\nu_f - 2\nu_i) + 35 (2\nu_f - \nu_i) \quad (4.245)
\]
\[
\eta_2 = 5\nu_f \left[ \mu_f / \mu_i - 8 \right] + 7 (\mu_f / \mu_i + 4) \quad (4.246)
\]
\[
\eta_3 = (\mu_f / \mu_i) (8 - 10\nu_i) + (7 - 5\nu_i) \quad (4.247)
\]

φ is given in equation (4.239).

Based on the Van der Poel’s formula for the shear modulus of a particulate composite, Smith (1974, 1975) also gave the condition for determining the effective shear modulus of the CSA as follows:
\[
\alpha \left( \frac{\mu^*}{\mu_i} - 1 \right)^2 + \beta \left( \frac{\mu^*}{\mu_i} - 1 \right) + \gamma = 0 \quad (4.248)
\]
where
\[
\alpha = \left[ 4P(7 - 10\nu_i) - S\phi^{7/3} \right] Q - (8 - 10\nu_i) (M - 1)\phi - 126 P (M - 1) \phi (1 - \phi^{2/3})^2 \quad (4.249)
\]
\[
\beta = 35 (1 - \nu_i) P \left[ Q - (8 - 10\nu_i) (M - 1)\phi \right] - 15 (1 - \nu_i) P (7 - 10\nu_i) - S \phi^{7/3} (M - 1)\phi \quad (4.250)
\]
\[
\gamma = -525 P (1 - \nu_i)^2 (M - 1)\phi \quad (4.251)
\]

with
\[
M = \mu_f / \mu_i \quad (4.252)
\]
\[
P = (7 + 5\nu_f) M + 4(7 - 10\nu_f) \quad (4.253)
\]
\[
Q = (8 - 10\nu_i) M + (7 - 5\nu_i) \quad (4.254)
\]
\[
S = 35 (7 + 5\nu_f) M (1 - \nu_i) - P (7 + 5\nu_i) \quad (4.255)
\]

φ is given in equation (4.239).
Equation (4.241) and equation (4.248) are verified as equivalent in the determination of the effective shear modulus of the CSA. Solving the above equations, one can determine the exact solution for the effective shear modulus of the CSA model. One of the roots is negative and is extraneous. The positive root provides the value of the effective shear modulus.

4.6.4 Effective Young’s Modulus and Poisson’s Ratio

Effective Young’s modulus and Poisson’s ratio for the CSA can be calculated from the well-known expressions:

\[
E^* = \frac{9k^* \mu^*}{3k^* + \mu^*} \quad (4.256)
\]

\[
v^* = \frac{3k^* - 2\mu^*}{6k^* + 2\mu^*} \quad (4.257)
\]

4.6.5 Numerical Examples

In order to illustrate the effects of imperfect interface and interphase thickness on the overall effective mechanical and thermal properties of CSA, we consider a special case of CSA that consists of spherical alumina trihydrate (ATH) particle and interphase with the following properties:

For particles:

\[E_f = 70\text{GPa}\]

\[v_f = 0.24\]

\[\alpha_f = 13 \times 10^{-6} / ^\circ\text{C}\]
For interphase

\[ v_i = 0.31 \]

\[ \alpha_i = 70 \times 10^{-6}/^\circ\text{C} \]

\[ \delta/r = 0.01 \text{ and } \delta/r = 0.001 \]

The nondimensional interface parameter is defined as \( q = E_i/E \). A zero value of \( q \) implies that there are no interface displacement jumps and the perfectly bonded interface conditions exist. At the other extreme, infinite value of \( q \) implies that the interface tractions do not exist and the filler is debonded from the adjoining matrix media. Finite positive values for \( q \) define an imperfect interface, which lies between two extreme cases mentioned above.

In this part of the dissertation, we focus on the effects of degradation of the interface bond from perfect bonding to completely debonding and the influence of the thickness of the interphase on the overall mechanical and thermal properties of the CSA. A plot of effective thermal expansion coefficient as functions of \( q \) is shown in figure 4.4 for different interphase thicknesses. Thickness of the interphase has a great influence on the overall effective CTE of CSA. It was observed that weakening the bond decreases the effective CTE until it asymptotically attains the CTE value of ATH. The reason for this is that when the interphase does not exist, the effective CTE of the material is exactly the CTE of the filler.
Figures 4.5-4.7 show the effects of the interphase bond modulus and thickness on the effective shear modulus, Young’s modulus, and bulk modulus. The stiffness of the bond has a strong effect on the degradation of the shear modulus, Young’s modulus, and bulk modulus. As the interface becomes thinner for the same $E_i$ value, the effective shear modulus increases. On the other hand for the same interphase thickness, as the elastic modulus value $E_i$ of the interphase decreases, the effective shear modulus decreases. This is also true for both the effective bulk modulus and Young's modulus. Figure 4.8 shows the effects of the interphase bond modulus and thickness on the effective Poisson's
ratio. Effective Poisson's ratio seems to be independent of the interphase stiffness when 
$q \leq 10^2$ and $q \geq 10^4$.

Figure 4.5 Variation of effective shear modulus with the interface parameter $q$
Figure 4.6 Variation of effective Young’s modulus with the interface parameter $q$
Figure 4.7 Variation of effective bulk modulus with the interface parameter $q$
We analytically and numerically evaluated the effective elastic properties and the thermal expansion coefficients of the composite sphere assemblage. All the previous results show that the bulk and shear moduli are insensitive to the value of the Poisson’s ratio of interphase. Numerical results also show that the nature of the interphase has significant effects on the stiffness and the thermal expansion coefficient of the CSA.
4.7 Micromechanical Model of Particulate Composites

The nature of the bond between particles and the matrix material has a significant affect on the mechanical behavior of particulate composites. Most analytical and numerical models assume that the bond between the filler and matrix is perfect and can be modeled using the continuity of tractions and displacements across a discrete interface. However, internal defects and imperfect interfaces are well known to exist in composites and the incorporation of such phenomena into the general theory requires modification and relaxation of the continuity of displacements between the constituents. The imperfect interface bond may be due to the compliant interfacial layer known as interphase or interface damage, which may have been created deliberately by coating the particles. It may also develop during the manufacturing process due to chemical reactions between the contacting particles and the matrix material or due to interface damage from cyclic loading. Moreover, the strength of the bond at the interface controls the mechanical response and fatigue life of the composite, (Basaran, Nie and Hutchins, 2004). By controlling the stress-strain response of the interphase, it is possible to control overall behavior of the composite.

In this dissertation, a powerful micromechanical model for particulate composites with CTE mismatch is proposed based on the works of Ju and Chen (1994a, 1994b) and Ju and Tseng (1996). Ju's micromechanical model for perfect interface particulate composites is well known as the most effective medium approach based on generalizations of the Eshelby method (Eshelby, 1957). This model would be particularly useful for situations with random microstructures. We incorporated the effects of CTE
mismatch and the imperfect interface between the particle and the matrix into the Ju’ model.

In our micromechanical model, particulate composites are treated as three-phase composites consisting of agglomerate of particles, the bulk matrix and the interfacial transition zone around the agglomerate as shown in figure 4.2. The interfacial transition zones are assumed to have perfect bonding with matrix and particles. The inner composite sphere assemblage (CSA), consisting of the particle and the interfacial transition zone, is regarded as an equivalent spherical particle with the effective mechanical and thermal properties determined in the former section. The constitutive models of particulate composite with perfect interface can be readily applied to the imperfect interface particulate composite. The detailed modeling procedure will be discussed in the next section.

4.7.1 Modeling Procedures for Particulate Composites

In this section, we will discuss the modeling procedures for a particulate composite, including how the interface properties, CTE mismatch between the particle and the matrix, and an isotropic damage parameter are introduced in this model.

The modeling process consists of four steps. The first step is the simplification of the real particulate composites, which is shown in figure 4.9. A is a representation of the real microstructure for a particulate composite, where particles have different sizes and shapes. In order to get an analytical expression for the effective behavior of the particulate composite, we must make some assumptions. For simplicity, we assume that the particles are uniform spherical with diameter of 35µm. From the SEM image of the
particles, we concluded that that is a reasonable assumption. The interfacial layer is used to model the imperfect interface condition. The displacement jumps are defined by the deformation of the interphase. The particulate composite is defined as a three-phase system that includes particles, the thin interphase and the matrix. The simplified microstructure for a particulate composite is shown as B in figure 4.9.

The simplified microstructure for the particulate composites includes the particle, the interphase and the matrix. But the state-of-the-art theory for the microstructure of a composite can not consider the interphase directly. In order to use the current theory for particulate composites with perfect interfacial bonding between the filler and the matrix, the particle and the interphase must be regarded as one, namely a particle-interphase assemblage. The microstructure of composite is now simplified as C shown in figure 4.9.
4.10. The microstructure of C includes the particle-interphase assemblage and the matrix. But we need the thermomechanical properties for the particle-interphase assemblage.

![Diagram](image)

Figure 4.10 Modeling procedures – step 2: equivalence

Finding the effective thermomechanical properties for the spherical particle-interphase assemblage is a must. Fortunately, former researchers have found the answers for us, which will be discussed in the following sections. Now the interfacial layer is coupled to the effective thermomechanical properties of the particle-interphase assemblage.
The particulate composite is simplified as a two-phase system with perfect interfacial bonding between the particle-interphase assemblage and the matrix. The current theories can be used for the proposed micromechanical models for a particulate composite with perfect interfacial bonding, which is discussed in previous section. Once the equivalent thermomechanical properties for the particulate composite are obtained, continuum damage mechanics can be used to analyze the damage behavior of the particulate composite, where the interfacial properties and CTE mismatch between the matrix and the filler are coupled. This final modeling step is shown in figure 4.12.
4.7.2 Elastic Properties of Particulate Composites

Based on Ju and Chen’s formulations (1994a, 1994b), the noninteracting solutions for the effective properties of the two-phase composite with imperfect bonding can be modified by substituting the properties of the particle with the properties of CSA:

\[
k = k_m \left\{ 1 + \frac{3(1 - v_m)(k^* - k_m)\phi_f}{3(1 - v_m)k_m + (1 - \phi_f)(1 + v_m)(k^* - k_m)} \right\}
\]

(4.258)

\[
\mu = \mu_m \left\{ 1 + \frac{15(1 - v_m)(\mu^* - \mu_m)\phi_f}{15(1 - v_m)\mu_m + (1 - \phi_f)(8 - 10v_m)(\mu^* - \mu_m)} \right\}
\]

(4.259)

Similarly, the pairwise interacting solutions for the effective properties of the two-phase composite with the imperfect bond can be modified as:

\[
k = k_m \left\{ 1 + \frac{30(1 - v_m)(3\gamma_1 + 2\gamma_2)\phi_f}{3\beta_1 + 2\beta_2 - 10(1 + v_m)(3\gamma_1 + 2\gamma_2)\phi_f} \right\}
\]

(4.260)
\[ \mu = \mu_m \left[ 1 + \frac{30(1-v_m)\gamma_2 \phi_f}{\beta_2 - 4(4-5v_m)\gamma_2 \phi_f} \right] \]  
(4.261)

where

\[ \beta_1 = 2(5v_m - 1) + 10(1-v_m) \left( \frac{k_m}{k^*-k_m} - \frac{\mu_m}{\mu^* - \mu_m} \right) \]  
(4.262)

\[ \beta_2 = 2(4-5v_m) + 15(1-v_m) \frac{\mu_m}{\mu^* - \mu_m} \]  
(4.263)

and

\[ \gamma_1 = \frac{5\phi_f}{8\beta_2^2} \left(13 - 14v_m\right)v_m - \frac{8\beta_1}{3\beta_1 + 2\beta_2} \left(1 - 2v_m\right)(1 + v_m) \]  
(4.264)

\[ \gamma_2 = \frac{1}{2} + \frac{5\phi_f}{16\beta_2^2} \left(25 - 34v_m + 22v_m^2\right) - \frac{6\beta_1}{3\beta_1 + 2\beta_2} \left(1 - 2v_m\right)(1 + v_m) \]  
(4.265)

where \( k^* \) and \( \mu^* \) are the effective bulk modulus and shear modulus of CSA, \( \phi_f \) is the particle volume fraction.

The composites studied in this work were prepared using lightly cross-linked poly-methyl methacrylate (PMMA) filled with alumina trihydrate (ATH). The following phase properties were used for the numerical analysis.

Particle: \( E_f = 70 \text{GPa} \), \( v_f = 0.24 \)

Matrix: \( E_m = 3.5 \text{GPa} \), \( v_m = 0.31 \)

Particle volume fraction is \( \phi_f = 0.48 \)

Nondimensional interface parameter is defined as \( q = E_f/E_i \)

Three kinds of composites with different interfacial properties were prepared.

Composite A has the strongest interfacial adhesion due to the addition of a special
adhesion promoting additives, where the value of the nondimensional interface parameter $q = E_f / E_i$ can be assumed to be 1. The interfacial adhesion strength of composite C is the weakest due to the addition of debonding promoting additives. The value of the nondimensional interface parameter $q$ for composite C can be assumed to be a very large number. The interfacial strength of the composite B is moderate. The value of nondimensional interface parameter $q$ for composite B can be assumed to be some value between that for composite A and composite C. The elastic Young's moduli for composite A, B and C are determined from the uniaxial tensile tests at a strain rate of $1 \times 10^{-4}$ sec$^{-1}$ according to ASTM D638-98.

The effects of the interphase properties on the effective Young’s modulus of two-phase composite are shown in figures 4.13-4.15, where the elastic properties of composites with different interphase properties obtained from test data were also plotted for comparison. These results indicate that the pairwise interacting solution yields a better approximation of the overall elastic modulus. Observation of figure 4.13, figure 4.14 and figure 4.15 also indicates that as the thickness of the interphase gets larger, the effective elastic modulus value decreases for the same $q$ value.
Figure 4.13 Effective Young’s modulus vs. interface parameter at volume fraction of 48% (The thickness of interphase is 1/10 of the diameter of particles)
Figure 4.14 Effective Young’s modulus vs. interface parameter at volume fraction of 48% (The thickness of interphase is 1/100 of the diameter of particles)
Figure 4.15 Effective Young’s modulus vs. interface parameter at volume fraction of 48% (The thickness of interphase is 1/1000 of the diameter of particles)

4.7.3 A Damage Coupled Viscoplastic Model for Particulate Composites

4.7.3.1 Loading Function

Viscoplastic yielding and flow occur only in the matrix, and the matrix determines the viscoplastic behavior of the composite. The magnitude of the current equivalent stress norm of the matrix can be utilized to determine the possible viscoplastic behavior in the composite. Regarding the composite as viscoplastic overall, when the ensemble-volume averaged stress norm in the matrix reaches a certain level, the effective loading function for the composite can be proposed as:

\[
 f(\sigma, \alpha) = \sqrt{(\sigma - \sigma^T) : \tilde{T} : (\sigma - \sigma^T)} - \sqrt{T^2 + 2T \sigma_y(\alpha)} 
\]  

(4.266)
where $\overline{\sigma}$ is the average stress in the particulate composite; $\sigma^T$ is the stress caused by the CTE mismatch between the matrix and the particle which is given by equation (190); $T$ is the fourth order tensor which is given by equation (4.211); $T_1$ and $T_2$ are given by equation (4.217) and equation (4.218), respectively; $\overline{\sigma}_s(\overline{\alpha})$ is the isotropic hardening function of the composite materials; $\overline{\alpha}$ is the equivalent viscoplastic strain that defines isotropic hardening of the yield surface of the composites,

$$\dot{\overline{\alpha}} = \sqrt{T_1 + 2T_2} \sqrt{\epsilon^v : T^{-1} : \epsilon^v}$$

(4.267)

The factors in the effective yield and the effective plastic strain increment equations are chosen so that the effective stress and effective plastic strain increments are equal to the uniaxial stress and uniaxial plastic strain increment in a uniaxial monotonic tensile test. It should be noted that the effective loading function is pressure dependent now and not of the von-Mises type any more. So the particles have significant effects on the viscoplastic behavior of the matrix materials.

In order to simulate damage behavior of composite materials, there is a need for introducing a damage parameter in the above proposed model. Damage mechanics provides us a basic framework to develop damage evolution models. According to the strain equivalence principle, the effective damage coupled loading function for an isotropic damage parameter $D$ can be written as,

$$f(\overline{\sigma}, \overline{\alpha}) = \sqrt{\frac{\overline{\sigma}}{1-D} - \overline{\sigma}^T} : \overline{T} : \left(\frac{\overline{\sigma}}{1-D} - \overline{\sigma}^T\right) - \sqrt{T_1 + 2T_2} \overline{\sigma}_s(\overline{\alpha})$$

(4.268)

It is obvious that the damage increases the equivalent stress norm of the composite, which tend to amplify the viscoplastic behavior of composite.
If the kinematic hardening behavior is included, let $\bar{\beta}$ define the center of the yield surface of the composite in the stress space, and the relative stress be defined as $\bar{\sigma} - \bar{\beta}$. Assume the particles have the same effects on the stress norm of the matrix as on the kinematic behavior of the matrix; the stress norm defining the viscoplastic behavior of the matrix can be updated as:

$$\langle H \rangle_n (x) = \left( \bar{\sigma} - \bar{\beta} - \bar{\sigma}' \right) : \bar{T} : \left( \bar{\sigma} - \bar{\beta} - \bar{\sigma}' \right)$$  \hspace{1cm} (4.269)

Therefore, the effective damage coupled loading function for the composite can be proposed as:

$$f(\bar{\sigma}, q) = \sqrt{\left( \frac{1}{1-D} \bar{\sigma} - \bar{\beta} - \bar{\sigma}' \right) : \bar{T} : \left( \frac{1}{1-D} \bar{\sigma} - \bar{\beta} - \bar{\sigma}' \right) - \sqrt{\bar{T}_i + 2\bar{T}_2 \left[ \sigma + K(\bar{\alpha}) \right]}}$$  \hspace{1cm} (4.270)

where $q = \{\bar{\alpha}, \bar{\beta}\}$ is chosen as the internal viscoplastic variable.

For simplicity, the Perzyna-type viscoplasticity model is employed to characterize rate (viscosity) effects in plastic materials here. Therefore, the effective ensemble-volume averaged plastic strain rate for the composite can be expressed as:

$$\dot{\varepsilon}^p = \gamma \frac{\partial f}{\partial \sigma} = \frac{1}{1-D} \gamma n$$  \hspace{1cm} (4.271)

where

$$n = \frac{\bar{T} : \left( \frac{1}{1-D} \bar{\sigma} - \bar{\beta} - \bar{\sigma}' \right)}{\sqrt{\left( \frac{1}{1-D} \bar{\sigma} - \bar{\beta} - \bar{\sigma}' \right) : \bar{T} : \left( \frac{1}{1-D} \bar{\sigma} - \bar{\beta} - \bar{\sigma}' \right)}}$$  \hspace{1cm} (4.272)

and $\gamma$ denotes the plastic consistency parameter

$$\gamma = \frac{\langle f \rangle}{\eta} = \frac{\langle f \rangle}{2\mu\tau}$$  \hspace{1cm} (4.273)
where \( \eta \) is viscosity coefficient, \( \tau \) is called relaxation time.

And the effective equivalent viscoplastic strain rate is defined as

\[
\dot{\alpha} = \sqrt{\frac{T_1 + 2T_2}{1 - D}} \frac{\gamma}{1 - D}
\]  

(4.274)

The evolution of the back stress, \( \overline{\beta} \), depends on the plastic strain or plastic work history. The earlier model for the evolution of the back stress is due to Prager (1956), and was subsequently modified by Ziegler (1959). The Prager hardening assumption is that during yielding the back stress increment \( d\overline{\beta} \) is equal to the component of \( d\sigma \) in the direction normal to the yield surface. Since the plastic strain increment is also normal to the yield surface, the increment \( d\overline{\beta} \) can be written as

\[
d\overline{\beta} = \left[ \frac{d\sigma}{d\varepsilon^p} \right] \frac{d\varepsilon^p}{d\varepsilon^p}
\]  

(4.275)

In the case of linear kinematic hardening, we have

\[
d\overline{\beta} = \frac{(T_1 + 2T_2)^{1.5}}{(T_1 + 2T_2)^2 + 2T_1^2} H' \dot{\alpha} n
\]  

(4.276)

where \( H' \) is the kinematic hardening modulus. The factor in equation (4.726) is chosen so that the effective stress and effective plastic strain increments are equal to the uniaxial stress and uniaxial plastic strain increment in a uniaxial monotonic tensile test.

4.7.3.2 Damage Evolution

The entropy production is a non-negative quantity based on irreversible thermodynamics and thus serves as a basis for the systematic description of the irreversible processes occurring in a solid. Isotropic damage evolution function based on
entropy has been discussed in chapter 3 of this dissertation. The damage parameter is defined as:

\[ D = D_{cr} \left[ 1 - e^{\frac{m - \Delta s}{R}} \right] \]  

(4.277)

where \( D_{cr} \) is a proportional critical damage coefficient, \( R \) is the gas constant, and \( \Delta s \) is the entropy production and can be calculated as follows:

\[ \Delta s = \int_{t_0}^{t} \sigma : \dot{\varepsilon}^{vp} dt + \int_{t_0}^{t} \left( \frac{k}{T^2 \rho} |\text{grad } T|^2 \right) dt + \int_{t_0}^{t} \frac{r}{T} dt \]  

(4.278)

where \( \rho \) is the density, \( T \) is temperature, \( k \) is termed the thermal conductivity of the composite, and \( r \) is the distributed internal heat source.

4.7.3.3 Computational Integration Algorithm

In this section, we employ the general return-mapping algorithms to solve the damaged coupled viscoplastic corrector problem proposed from equation (4.270) to equation (4.278). The general return-mapping algorithm was proposed by Simo and Taylor (1985) and summarized in details by Simo and Hughes (1998). In order to minimize confusion, the symbol \( \Delta \) is used to denote an increment over a time step, or an increment between successive iterations. For the rate-of-slip \( \gamma \), we adhere to the conventions: \( \Delta \gamma = \gamma \Delta t \) denotes the increment of \( \gamma \) over a time step, and \( \Delta^2 \gamma \) denotes the increment of \( \Delta \gamma \) between iterations.

Let \( C \) be the elastic consistent tangent moduli of the particulate composite, then the overall stress-strain relationship can be written as:

\[ \sigma_{n+1} = (1 - D) C : (\varepsilon_{n+1}^{vp} - \varepsilon_{n+1}^b - \varepsilon_{n+1}^h) \]  

(4.279)
Since $\varepsilon_{n+1}$ and $\varepsilon_{n+1}^{th}$ is fixed during the return-mapping stage, it follows that:

$$\Delta \varepsilon^{vp} = -\frac{1}{1-D} C^{-1} \Delta \sigma$$  \hspace{1cm} (4.280)

From equation (4.277), we have

$$\dot{D} = \frac{D_{cr} m}{R} \exp \left( -\frac{m}{R} \Delta s \right) \Delta s$$  \hspace{1cm} (4.281)

Assuming that the heat generated within the system by external agencies (inductive heating, for example) is negligible, so the distributed internal heat source of strength per unit mass $r$ is zero. Therefore, we have from equation (4.278) for the isothermal process at each increment:

$$\Delta \dot{s} = \frac{\sigma \varepsilon^{vp} r}{T \rho} + \frac{r}{T}$$  \hspace{1cm} (4.282)

Using equations (4.280) and (4.282), equation (4.281) becomes

$$\Delta D = -\frac{1}{1-D} \frac{D_{cr} m}{T \rho R} \exp \left( -\frac{m}{R} \Delta s \right) \sigma C^{-1} \Delta \sigma$$  \hspace{1cm} (4.283)

From equations (4.271), (4.274) and (4.276), we also have

$$\varepsilon_{n+1}^{vp} = \varepsilon_{n}^{vp} + \frac{1}{1-D} \Delta \gamma \varepsilon$$  \hspace{1cm} (4.284)

$$\alpha_{n+1} = \alpha_{n} + \frac{1}{1-D} \sqrt{T_{1} + 2T_{2}} \Delta \gamma$$  \hspace{1cm} (4.285)

$$\overline{\beta}_{n+1} = \overline{\beta}_{n} + \left( \frac{T_{1} + 2T_{2}}{T_{1} + 2T_{2}} \right)^{1.5} \Delta H \varepsilon$$  \hspace{1cm} (4.286)

Let

$$m_{i} = \sqrt{T_{1} + 2T_{2}}$$  \hspace{1cm} (4.287)

164
\[ m_2 = \frac{(\bar{T}_i + 2\bar{T}_2)^{1.5}}{(\bar{T}_i + 2\bar{T}_2)^2 + 2\bar{T}_i^2} \] (4.288)

\[ m_3 = -\frac{D_m m_e}{T \rho R} \exp\left(-\frac{m_s}{R} \Delta s\right) \] (4.289)

Also we have

\[ \frac{\partial f}{\partial \sigma} = \frac{1}{1 - D} n \] (4.290)

\[ \frac{\partial^2 f}{\partial \sigma^2} = \frac{1}{(1 - D)^2} N \] (4.291)

\[ \frac{\partial f}{\partial \beta} = -n \] (4.292)

\[ \frac{\partial^2 f}{\partial \beta^2} = N \] (4.293)

\[ \frac{\partial f}{\partial D} = \frac{n : \sigma}{(1 - D)^2} \] (4.294)

\[ \frac{\partial f}{\partial \alpha} = -m_i K' \] (4.295)

\[ \frac{\partial n}{\partial \beta} = -N \] (4.296)

\[ \frac{\partial n}{\partial \sigma} = \frac{1}{1 - D} N \] (4.297)

\[ \frac{\partial n}{\partial D} = \frac{1}{(1 - D)^2} N : \sigma \] (4.298)

where \( K' = \frac{\partial \bar{\sigma}}{\partial \bar{\alpha}} \) is the isotropic hardening modulus.
We define the following residual functions as follows:

\[ R_{\alpha} = -\alpha_{n+1} + \alpha_n + \frac{m_1}{1-D} \Delta \gamma \]  
(4.300)

\[ R_{\gamma} = \frac{2\mu \tau \Delta \gamma}{\Delta t} - \langle f \rangle \]  
(4.301)

\[ R_{\varepsilon} = -\varepsilon^n_{\alpha\varepsilon} + \varepsilon^n_{\gamma\varepsilon} + \frac{1}{1-D} \Delta \gamma \mathbf{n} \]  
(4.302)

\[ R_{\beta} = -\beta_{n+1} + \beta_n + m_2 \Delta H \mathbf{n} \]  
(4.303)

Literalizing these residual functions, we have

\[ R_{\alpha} - \Delta \alpha_{n+1} + \frac{m_1}{1-D} \Delta^2 \gamma + \frac{m_1 m_3}{(1-D)^3} \Delta \gamma \sigma \mathbf{C}^{-1} \Delta \sigma = 0 \]  
(4.304)

\[ \mathbf{n}' \Delta \sigma - \mathbf{n} \Delta \beta = R_{\gamma} + m_1 K' R_{\alpha} + \left( \frac{m_1^2 K'}{1-D} + 2\mu \frac{\tau}{\Delta t} \right) \Delta^2 \gamma \]  
(4.305)

\[ \mathbf{P} : \Delta \sigma - \mathbf{Q} : \Delta \beta + \frac{\Delta^2 \gamma}{1-D} \mathbf{n} + R_{\varepsilon} = 0 \]  
(4.306)

\[ \mathbf{R} : \Delta \sigma - \mathbf{S} : \Delta \beta + \frac{m_1 m_2}{1-D} H' \Delta^2 \gamma \mathbf{n} + m_2 H' R_{\alpha} \mathbf{n} + R_{\beta} = 0 \]  
(4.307)

where

\[ \mathbf{P} = \frac{1}{1-D} \left[ \mathbf{C}^{-1} + \frac{\Delta \gamma}{1-D} \mathbf{N} + \frac{\Delta \gamma m_1}{(1-D)^2} \left( \frac{\mathbf{N} \sigma}{1-D} + \mathbf{n} \right) \otimes (\sigma \mathbf{C}^{-1}) \right] \]  
(4.308)

\[ \mathbf{Q} = \frac{\Delta \gamma}{1-D} \mathbf{N} \]  
(4.309)
\[ R = \frac{m_2}{1-D} \left[ \Delta HN + \frac{m_3}{(1-D)^2} (\Delta HN \sigma + m_1 H' \Delta \gamma n) \otimes (\sigma C^{-1}) \right] \] (4.310)

\[ S = I + m_2 \Delta HN \] (4.311)

\[ n' = \frac{1}{1-D} \left[ n + \frac{m_3}{(1-D)^2} (n \bar{\sigma} - m_1^2 K' \Delta \gamma) (\bar{\sigma} C^{-1}) \right] \] (4.312)

Combining equations (4.306) and (4.307),

\[
\begin{bmatrix}
P & Q \\
R & S
\end{bmatrix}
\begin{bmatrix}
\Delta \bar{\sigma} \\
-\Delta \bar{\beta}
\end{bmatrix}
+ \begin{bmatrix}
\Delta^2 \gamma \\
1
\end{bmatrix}
\begin{bmatrix}
m_1 m_2 H' \\
m_2 H'R_n + R_n'
\end{bmatrix}
+ \begin{bmatrix}
R_x \\
m_2 H' R_n + R_n'
\end{bmatrix}
= 0
\] (4.313)

From equations (4.313) and (4.305), we have

\[
\Delta^2 \gamma = \frac{-R_f - m_1 K' R_n - [n' \cdot n] A \begin{bmatrix}
R_x \\
m_2 H' R_n + R_n'
\end{bmatrix}}{\frac{m_1^2 K'}{1-D} + 2 \mu \frac{\tau}{\Delta t} + \frac{1}{1-D} [n' \cdot n] A \begin{bmatrix}
n \\
m_2 m_2 H' n
\end{bmatrix}}
\] (4.314)

where

\[
A^{-1} = \begin{bmatrix}
P & Q \\
R & S
\end{bmatrix}
\] (4.315)

\[
A = \begin{bmatrix}
\tilde{P} & \tilde{Q} \\
\tilde{R} & \tilde{S}
\end{bmatrix}
\] (4.316)

\[
\tilde{P} = \left( P - Q \cdot S^{-1} \cdot R \right)^{-1}
\] (4.317)

\[
\tilde{Q} = -\left( P - Q \cdot S^{-1} \cdot R \right)^{-1} \cdot (Q \cdot S^{-1})
\] (4.318)

\[
\tilde{R} = -\left( S^{-1} \cdot R \right) \cdot \left( P - Q \cdot S^{-1} \cdot R \right)^{-1}
\] (4.319)

\[
\tilde{S} = S^{-1} + \left( S^{-1} \cdot R \right) \cdot \left( P - Q \cdot S^{-1} \cdot R \right)^{-1} \cdot (Q \cdot S^{-1})
\] (4.320)

So we have
\[
\begin{aligned}
\begin{bmatrix}
\Delta \sigma \\
-\Delta \beta
\end{bmatrix} &= -A \begin{bmatrix}
\frac{\Delta^2 \gamma}{1-D} n + R_e \\
\left( \frac{m_1 \Delta^2 \gamma}{1-D} + R_\alpha \right) m_z H' n + R_\beta
\end{bmatrix} \\
\Delta \bar{e}^{vp} &= -\frac{1}{1-D} C^{-1} \Delta \bar{\sigma} \\
\Delta^2 s &= \frac{\bar{\sigma} \Delta \bar{e}^{vp}}{T \rho} \\
\Delta s_{n+1} &= \Delta s_n + \Delta^2 s \\
\Delta D_{n+1} &= -m_3 \left( \bar{\sigma}_{n+1} \Delta \bar{e}^{vp} \right) \\
\Delta \alpha_{n+1} &= R_\alpha + \frac{m}{1-D} \Delta^2 \gamma - \frac{m_3}{(1-D)^2} \Delta \gamma \sigma \Delta \bar{e}^{vp}
\end{aligned}
\] (4.321)

Then, we update the viscoplastic strain, consistency parameter, stress, damage parameter and entropy production and effective equivalent viscoplastic strain, and iterate until the norms of residual functions (4.300), (4.301), (4.302) and (4.303) become small enough. In the program, it was assumed that the converging results are achieved when the norms of these residual functions are all equal to or less than $1 \times 10^{-5}$.

The procedure summarized above is simply a systematic application of Newton’s method to the system of equations (4.270) to (4.278) that results in the computation of the closest point projection from the trial state onto the yield surface. A geometric interpretation of the iteration scheme is contained in figure 4.16.

It should be noted that the general return-mapping algorithm is unconditionally stable and the convergence of the algorithms toward the final value of the state variable is obtained at a quadratic rate. The further information on the general return-mapping algorithm is given in Simo and Hughes (1998), Ortiz and Martin (1989).
4.7.3.4 Consistent Elastoviscoplastic Tangent Modulus

An important advantage of the algorithm lies in the fact that it can be exactly linearized in closed form. This leads to the notion of a consistent elastoviscoplastic tangent moduli.

Let \( C \) be the elastic consistent elastoviscoplastic tangent moduli, then the increment stress-strain relationship can be written as:

\[
\sigma = (1 - D) C (\varepsilon - \varepsilon^n) \tag{4.327}
\]

Differentiating equation (4.277) and equation (4.278), we have

\[
d \sigma = (1 - D) C (d \varepsilon - d \varepsilon^n) \tag{4.328}
\]

Where \( m_3 \) is given by equation (4.289).

Differentiating equation (4.284), we have
\[
d\varepsilon^p = \frac{\Delta \gamma}{(1-D)^2} WNd\bar{\sigma} - \frac{\Delta \gamma}{1-D} WNd\bar{\beta} + \frac{d\Delta \gamma}{1-D} Wn \tag{4.329}
\]

where
\[
W^{-1} = I + \frac{\Delta \gamma \gamma_3}{(1-D)^2} \left( \frac{N\sigma}{1-D} + n \right) \otimes \sigma \tag{4.330}
\]

Differentiating equation (4.285), we have
\[
d\alpha = \frac{m_1}{1-D} d\Delta \gamma - \frac{m_3}{(1-D)^2} \Delta \gamma \bar{\sigma} d\varepsilon^p \tag{4.331}
\]

Differentiating equation (4.286), we have
\[
d\bar{\beta} = -\frac{m_2 m_1 \Delta H}{(1-D)^3} (N\sigma \otimes \sigma) d\varepsilon^p + \frac{m_1 \Delta H}{1-D} Nd\bar{\sigma} - m_2 \Delta HNd\bar{\beta} + m_2 nH' d\alpha \tag{4.332}
\]

Differentiating equation (4.273), we have
\[
\frac{1}{1-D} nd\bar{\sigma} - n d\bar{\beta} - \frac{m_1}{(1-D)^2} (n\bar{\sigma} - m_1^2 K \Delta \gamma) \bar{\sigma} d\varepsilon^p = \left( \frac{2\mu}{\Delta \tau} + \frac{m_2^2 K'}{1-D} \right) d\Delta \gamma \tag{4.333}
\]

From equations (4.327) and (4.329)
\[
p : d\bar{\sigma} - q : d\bar{\beta} + \frac{Wn}{1-D} d\Delta \gamma = d\varepsilon \tag{4.334}
\]

where
\[
p = \frac{1}{1-D} \left( C^{-1} + \frac{\Delta \gamma}{1-D} WN \right) \tag{4.335}
\]
\[
q = \frac{\Delta \gamma}{1-D} WN \tag{4.336}
\]

From equations (4.329), (4.331) and (4.332), we have
\[
r : d\bar{\sigma} - s : d\bar{\beta} + \frac{m_1 m_2 H'}{1-D} Wnd\Delta \gamma = 0 \tag{4.337}
\]

where

170
\[
\mathbf{r} = \frac{1}{1-D} \left( m_2 \Delta H N \mathbf{V W N} + \frac{\Delta \gamma}{1-D} \right) \\
\mathbf{s} = \mathbf{I} + m_2 \Delta H N \mathbf{V W N} + \frac{\Delta \gamma}{1-D} \\
V = - \frac{m_1 m_2}{(1-D)^3} H' \Delta \gamma \left[ \mathbf{N} \sigma + \mathbf{n} \right] \otimes \sigma
\]

Combining equations (4.334) and (4.337)
\[
\begin{bmatrix}
p & q \\
r & s
\end{bmatrix}
\begin{bmatrix}
\frac{d\mathbf{\bar{\sigma}}}{dt} \\
-d\mathbf{\bar{\beta}}
\end{bmatrix}
+ \begin{bmatrix}
\mathbf{W n} \\
\frac{1}{1-D} \mathbf{m}_1 \mathbf{m}_2 H'
\end{bmatrix}
\begin{bmatrix}
d\Delta \gamma \\
0
\end{bmatrix}
\]

Combining equations (4.329) and (4.333), we have
\[
\frac{n^*}{1-D} d\mathbf{\bar{\sigma}} - n^* d\mathbf{\bar{\beta}} = m_4 d\Delta \gamma
\]

where
\[
n^* = n - \frac{m_3 \Delta \gamma}{(1-D)^3} \left( n \mathbf{\bar{\sigma}} - m_1^2 K' \Delta \gamma \right) \left( \mathbf{\bar{\sigma}} \mathbf{W N} \right)
\]

\[
m_4 = \frac{m_3}{(1-D)^3} \left( n \mathbf{\bar{\sigma}} - m_1^2 K' \Delta \gamma \right) \left( \mathbf{\bar{\sigma}} \mathbf{W N} \right) + 2 \mu \frac{\tau}{\Delta t} + m_1^2 K' \frac{\Delta t}{1-D}
\]

From equations (4.341) and (4.342), we have
\[
d\Delta \gamma = \frac{n^* \left( \frac{1}{1-D} \mathbf{p} + \mathbf{\hat{r}} \right) d\mathbf{\varepsilon}}{m_4 + \frac{1}{1-D} \left[ \begin{bmatrix} n^* \\ n^* \end{bmatrix} \mathbf{a} \left( \begin{bmatrix} \mathbf{W n} \end{bmatrix} m_1 m_2 H' \mathbf{W n} \right) \right]}
\]

where
\[
\mathbf{a}^{-1} = \begin{bmatrix}
p & q \\
r & s
\end{bmatrix}
\]
a = \begin{bmatrix} \dot{p} & \dot{q} \\ \ddot{r} & \ddot{s} \end{bmatrix} \quad (4.347)

From equations (4.334) and (4.337), we have

\[ d\vec{\sigma} = \dot{\vec{p}} d\varepsilon - \left( \frac{1}{1 - D} \dot{\vec{p}} + \ddot{\vec{r}} \right) W_n d\Delta \gamma \quad (4.348) \]

From equations (4.345) and (4.348), we have

\[ C = \frac{d\vec{\sigma}}{d\varepsilon} = \dot{\vec{p}} - \frac{1}{m_4 + \frac{1}{1 - D} \left( \frac{n^*}{n^*} \right) W_n} \left\{ \frac{1}{1 - D} \dot{\vec{p}} + \ddot{\vec{r}} \right\} \quad (4.349) \]
CHAPTER 5

Experiments

5.1 Introduction

The composite studied in this project is prepared by casting and polymerizing a dispersion of ATH in PMMA. The compositions of the resulting composite is as follows: the matrix is lightly cross-linked poly-methyl methacrylate (PMMA) with a glass transition temperature of about 100 °C, and the filler is alumina trihydrate (ATH) agglomerates which is composed of many smaller ATH particles. The volume fraction of the filler particles and the average particle size of ATH were kept constant during the study, where only the interfacial strength was varied.

The test samples with different interfacial adhesion properties were prepared by DuPont Surfaces, Buffalo, NY. Different adhesion promoting and debonding promoting agents were tried. Table 5.1 shows the chemical and physical compositions of the tested specimens. Composite A has the strongest interfacial adhesion among the three composites due to the addition of a adhesion promoting additive. The interfacial adhesion strength of C is the weakest among the three composites due to the debonding additive agent applied to the surface of the filler ATH agglomerate. The interfacial strength of the composite B is moderate and is between the interfacial strength of composite A and composite C.
The properties of the particulate composites were determined experimentally through both Nano indentation tests and traditional mechanical tests. This chapter represents all the results and relevant test data obtained from the various tests, studies and investigations carried out in this project. Many factors related to particulate composites are often difficult to measure or separately experimentally. Thus, it is not surprising that there is a lot of scatter in experimental data on particle filled composite systems. Therefore it makes sense that it is difficult to obtain universal findings that are true for all particle filled composites. Also, the agreement between theory and experiment is often not very good.

This chapter aims to provide a better understanding of the material by giving detailed explanations where possible, and accounting for key experimental aspects associated with the material, and the effects of certain factors, test conditions and variables on exhibited behavior and properties. Furthermore, development of a damage
mechanical model is not possible without some degree of understanding of the failure process and availability of some experimental data.

5.2 Experimental Procedures

5.2.1 Nano Indentation Tests

Known as depth-sensing indentation, Nano indentation employs a high-resolution actuator to force an indenter into a test surface, and a high-resolution sensor to continuously measure the resulting penetration. Based on the indentation load-displacement data, it can measure the material properties such as hardness and the Young’s modulus. Nano indentation is ideal for mechanically characterizing small volumes of material, thin film, and surface coating layer. Nano indentation is ideal for measuring mechanical properties of composite materials (Basaran and Jiang, 2002).

Three sets of experiments were performed using the Nano indenter® XP on three orthogonal polished sections for measurement of the modulus and hardness in the three directions, respectively. This specimen is shown in figure 5.1.

![Figure 5.1 Specimen geometries for Nano Indentation tests (mm)](image)
5.2.2 Mechanical Tests

The tension, compression, creep and fatigue tests were undertaken in a servo-mechanical MTS machine type 858 table top system (10 kN capacity) controlled by a computer and fitted with an ATS 7510 box thermal chamber for the control of temperature. This test system has load, stroke and strain control capacity. The accuracy of temperature control was about +/- 1 °C and was monitored by using an ATS feedback control system and a thermocouple. The test system also includes an interchangeable 685.22 side-loading hydraulic wedge grip system with grip pressure up to 3000 psi. The hydraulically actuated grip system is independently activated and could maintain an adjustable grip force on the specimen grip face without backlash. Grips are attached to the load frame via a fixed, but adjustable, commercially available alignment system. The MTS 634.25 axial extensometer (from +50% to –10%) with the gauge length of 25.4 mm was used to measure uniaxial strain in the testing. The experiments were conducted as a function of strain rate and temperature for uniaxial tensile and compressive tests. The strain rate ranged from $1 \times 10^{-3}$ to $1 \times 10^{-5}$ sec$^{-1}$, and temperatures varied from room temperature to 90 °C. The specimen geometry used in these tests is shown in figure 5.2, which was cut from a plate. The details of the procedures used are described in the ASTM D 638-98 (1999). Great care was taken to reduce the experimental errors, which can arise from poor specimen alignment, thermal distortion of the strain extensometer arms, nonuniform heating of the test specimen, and variation in the initial loading rate.
5.3 Results and Discussions

5.3.1 Failure Mechanism of Particulate Composites

The acrylic particulate composite is known to accumulate considerable scattered microscopic damage in its service life. The compression and shear strength of the particulate composites is improved; however fillers often decrease the tensile strength and fatigue life. This low tensile stress and unfavorable combination of such properties as low thermal conductivity and relative high Young’s modulus of elasticity render acrylic particulate composites highly susceptible to failure under a service loading condition which promotes the generation of high magnitude thermal stress. The mechanical behavior of particulate composites is significantly affected by the nature of the bond between particles and the matrix material. The main aim of this work is to investigate the mechanisms of failure in PMMA/ATH composite using in situ observations during mechanical loadings at different temperatures and strain rates.

It is well established that the fracture of particulate composites is associated with interfacial debonding between the matrix and particles, particle cracking or particle-agglomerate breakage, and the ductile plastic failure in the matrix depending on the

Figure 5.2 Specimen geometries for mechanical tests (mm)
relative stiffness and strength of the two constituent materials and the interface strength. If both constituent materials have material properties in the same order of magnitude or the strength of the particles is low, particle cracking can occur. On the other hand, if the embedded particles are much stiffer and stronger than the matrix, matrix cracking (or cavity formation) and particle/matrix interface debonding become the major damage modes. However, the importance of interfacial strength in the fatigue life is not clear, and has not studied in great detail.

Most research regarding particulate composites assumes perfect adhesion between the filler and the polymer matrix as well as perfect dispersion of the individual filler particles. In fact, in the composite studied in this project the individual fillers are not separated from one another and wetted individually by the matrix phase; instead, the fillers are often agglomerates made up of many smaller particles, which is clearly seen in figure 5.3 and figure 5.4 in case of PMMA/ATH acrylic casting dispersion. These images are taken using scanning electronic microscope (SEM).

![Figure 5.3 Polished surface of composite A (gray regions are particles)](image)

Figure 5.3 Polished surface of composite A (gray regions are particles)
It is observed as shown in figure 5.5 that a macroscopic fracture initiates in the clusters of the reinforcing particles when there is strong interfacial bond between the reinforcing particles and the matrix, as in the case of material A. For weak interfacial bonding strength in the case of composite C, the macroscopic fracture is initiated by separation of the reinforcing particles from the matrix. The final fracture is produced by the incapacity of the matrix to carry loads released by the broken clusters of reinforcing particles.

The tensile fracture surfaces of the composite A at various temperatures are shown in figures 5.5 to figure 5.8. The tensile fracture surfaces of the composite B at various temperatures are shown in figures 5.9 to 5.11. The fracture surfaces of composite C at various temperatures are shown in figures 5.12 to figure 5.14. These fracture
surfaces testify that the interfacial strength has a great influence on the damage mechanism of particulate composites. Upon loading, the agglomerates of the ATH particles broke first in composite A, but for composite C, the agglomerates were pulled out from the PMMA matrix. Composite B exhibits a failure mode dominated by breaking of filler particles and pulling out of filler particles from the matrix.

In the case of composite A, the jagged surfaces observed in ATH particles indicated that ATH particles crack internally, rather than debonding at the interface due to the strong interfacial bond between the filler and the matrix. ATH filler particles are made up of small very jagged shaped crystals. ATH on its own is extremely hard and brittle with a very high recrystallization temperature (approximately couple of thousand degrees in Celsius). We or the manufacturer have not been able to measure the intergranular tensile strength of ATH particles. Yet, based on our extensive testing and SEM images we feel comfortable assuming that for composite A, the bonding strength between the particle and the matrix is stronger than the intergranular strength of the ATH particles. In the case of composite C, relatively smooth surfaces of ATH particle surfaces in composite C indicate that the filler particles are debonded without breaking internally. When the filler particles are almost completely debonded, the load is primarily carried by the matrix. Agglomerate filler particles are pulled out of the matrix rather than broken internally (crack between crystals) in composite C, we surmise, because of the fact that the interfacial bond between the filler particles and PMMA matrix is stronger than the intergranular tensile strength of the ATH agglomerates particles. In the case of the composite B, we observed a mixture of broken and pulled out particles, with most of the filler particles are broken internally.
Figure 5.5 Tensile fracture surfaces of composite A at room temperature

Figure 5.6 Tensile fracture surfaces of composite A at 50 °C
Figure 5.7 Tensile fracture surfaces of composite A at 75 °C

Figure 5.8 Tensile fracture surfaces of composite A at 90 °C
Figure 5.9 Tensile fracture surfaces of composite B at room temperature

Figure 5.10 Tensile fracture surfaces of composite B at 50 °C
Figure 5.11 Tensile fracture surfaces of composite B at 75 °C

Figure 5.12 Tensile fracture surfaces of composite C at room temperature
Figure 5.13 Tensile fracture surfaces of composite C at 50 °C

Figure 5.14 Tensile fracture surfaces of composite C at 75 °C
After the agglomerates were pulled out or broken internally, the force carried by the filler particle ATH is transferred to the matrix. The PMMA will deform more than the ATH dose, so that elliptical cavities or voids develop around each filler particle. When the transferred force is too high to be carried by the matrix alone, the specimen fails suddenly in a brittle manner for composite A and B. Composite C fails in a ductile manner, indicating there is little if any contribution from the filler particles. Application of strain in the last region of the uniaxial tensile tests is only to stretch the PMMA and enlarge existing cavities, which is believed to cause the volume growth during loading. Such a phenomenon has been studied by many researchers such as Ravichandran and Liu (1995), Kwon, Lee and Liu (1997, 1998). These studies investigated the nonlinear constitutive response of a damaged particulate composite in terms of the change in volume dilation and showed that the stress-strain response is nearly linear when there is little or no volume dilatation and the non-linearity sets in once the dilatation becomes significant.

The mechanism of the microdamage process in composite A and composite B may be thought of as a phenomenon passing at least through two different stages of damage, the first being the breaking up of aggregates of ATH and the second being properly the fracture of the matrix, which is shown in figure 5.15. The mechanism of microdamaging process in composite C may also be thought of as a phenomenon passing at least through two different stages of damage: the first being the adhesive debonding of the matrix from the filler and the second being the fracture of the matrix as shown figure 5.16 (Moshev and Evlampieva, 1997). Clearly, the debonding or particles cracking diminishes the resistance of the structural element. However, the latter retains a capability
to resist the extension for some time, although at a lower modulus. Only after the matrix part of the element has been broken may one consider that resistance has vanished.

Figure 5.15 Schematic of microdamage evolution in composite A and composite B

Figure 5.16 Schematic of microdamage evolution in composite C (Moshev and Evlampieva, 1997)

5.3.2 Nano Indentation Tests

Using the basic hardness, modulus, tip calibration and load control method, three sets of experiments were performed using the Nano Indenter® XP on three polished orthogonal sides of a cube made of particulate composite A. The elastic modulus and hardness were measured in the three orthogonal directions. For these tests, the allowable
The drift rate is 0.1 nm/s, and the maximum load was 250 mN. Table 5.2 and table 5.3 list the results of Nano Indenter® test for composite A at room temperature.

Table 5.2 Young’s modulus of composite A at room temperature from Nano Indenter® tests

<table>
<thead>
<tr>
<th></th>
<th>Modulus (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Side 1</td>
<td>Mean 9.368</td>
</tr>
<tr>
<td></td>
<td>Std. Dev. 1.999</td>
</tr>
<tr>
<td></td>
<td>% COV 21.34</td>
</tr>
<tr>
<td>Side 2</td>
<td>Mean 9.079</td>
</tr>
<tr>
<td></td>
<td>Std. Dev. 0.974</td>
</tr>
<tr>
<td></td>
<td>% COV 10.73</td>
</tr>
<tr>
<td>Side 3</td>
<td>Mean 9.257</td>
</tr>
<tr>
<td></td>
<td>Std. Dev. 0.991</td>
</tr>
<tr>
<td></td>
<td>% COV 10.17</td>
</tr>
</tbody>
</table>

Table 5.3 Hardness of composite A at room temperature from Nano Indenter® tests

<table>
<thead>
<tr>
<th></th>
<th>Hardness (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Side 1</td>
<td>Mean 0.264</td>
</tr>
<tr>
<td></td>
<td>Std. Dev. 0.036</td>
</tr>
<tr>
<td></td>
<td>% COV 13.49</td>
</tr>
<tr>
<td>Side 2</td>
<td>Mean 0.231</td>
</tr>
<tr>
<td></td>
<td>Std. Dev. 0.010</td>
</tr>
<tr>
<td></td>
<td>% COV 4.12</td>
</tr>
<tr>
<td>Side 3</td>
<td>Mean 0.240</td>
</tr>
<tr>
<td></td>
<td>Std. Dev. 0.021</td>
</tr>
<tr>
<td></td>
<td>% COV 8.79</td>
</tr>
</tbody>
</table>

These results show that the mechanical properties for composite A are almost the same in all the 3 directions, and composite A can be regarded as an isotropic material. The Young’s modulus measured using Nano indenter tests are also comparable with that obtained by uniaxial tensile tests as shown in the figure 5.17.
5.3.3 Monotonic Uniaxial Tests

Uniaxial tensile and compressive tests were carried out with the dog-bone shaped specimens having a 150 mm overall length and a 32 mm gauge length as shown in figure 5.2. Because the composite is brittle at room temperature and is sensitive to the preexisting flaws, Duck® tape was used on the specimen at the areas where the extensometer was clipped, to protect the specimen from flaws introduced by the blade of the extensometer. Great care was taken to reduce the experimental errors which can arise from poor specimen alignment, thermal distortion of the strain extensometer arms, nonuniform heating of the test specimen, and variation in the initial loading rate.
5.3.3.1 Influence of Strain Rates

Typical stress-strain curves obtained from the uniaxial tensile tests for composite A and composite C at room temperature are shown in figures 5.18 and figure 5.19 for several strain rates, where the influence of interfacial bonding strength on the composite strength are well demonstrated. The observations show that failure of the composite in tensile loading occurs in several stages. The stress-strain curve is initially linear elastic to a critical stress then it starts to behave nonlinearly. After the continuous nonlinear behavior, the stress-strain curve reaches the peak point and the failure of the specimen occurs suddenly without advance warning. At room temperature, composite A shows a brittle behavior and a high value of elastic modulus (relative to the matrix of the composite, PMMA). The failure behavior of particulate composites includes partial filler debonding or breaking up of agglomerates and progressive debonding or breaking up from the largest to smallest fillers throughout the strain history (Wong and Ait-Kadi, 1997). The initial elastic region of the curve was controlled primarily by the initial inclusion concentration and the matrix properties. Application of strain in the last region of the curve was only to stretch the binder and enlarge existing cavities. The nonlinear behavior of the stress-strain curve contributes to the microdamage (i.e. cavity formation) in the material. In this aspect, the starting point of the nonlinear stress-strain curve can be considered as the point of significant damage initiation while the peak stress point denotes the damage saturation. The damage increases between the two points. It was recognized early that volume dilation was closely linked to the nonlinear behavior which a particulate composite exhibited as it was loaded. This volume dilatation results from the microdamage in the particulate composite during continuous deformation. It was believed
that the stress-strain curve also starts to behave nonlinearly at the point where the volume dilatation begins (Ravichandran and Liu, 1995). The elastic modulus in tension also has strong amplitude dependence in which above critical amplitude of stress (or strain) the modulus shows a rapid decrease.

![Stress-strain curve](image)

Figure 5.18 Uniaxial tensile stress-strain curves of composite A at room temperature for different strain rates until failure

It should be pointed out that failure of composite A happens at strain of 0.8% compared to the strain of 2% in the case of composite C. Therefore, it is safe to say that strong interfacial bond between the filler and the matrix reduces the ductility greatly. Low ductility is usually associated with short fatigue life.
Another important effect of the strain rate on these stress-strain curves is that the material stiffness increased as the strain rate increased. Further, the material strength increased along with the increase of the strain rate. As the applied strain rate increased, the specimen is able to a greater stress under the same applied strain level. The comparison between the average stress-strain curves under the high and low strain rates also indicated that the low strain rate loading broke the linearity of stress-strain relation at a smaller applied strain than the high strain rate loading. This meant that the damage initiated at a smaller strain for the low strain rate loading.

Typical stress-strain curves obtained from the compressive tests for composite A and composite C are shown in figure 5.20 and figure 5.21 for different strain rates. Figure 5.22 shows the compressive stress-strain curve of the composite at displacement control.
rate 5e-3 and room temperature until failure (buckling). A similar trend was observed with the tensile tests except that the compressive strength is much larger than that in tension. Yield stress in tension is two to three times lower than the yield stress in compression.

Comparison of the stress-strain curves between tension and compression shows that the particulate composite exhibits markedly different inelastic behavior in tension and compression, which may be due to the different acting mechanism of reinforcing particles in tension and compression. The microstructure of the composite consists of a distribution of ATH agglomerates in a PMMA matrix. In tension, the ATH agglomerates act as stress concentrators, while in compression the flake serves to transmit stresses. The resulting material is brittle in tension, but in compression it is similar in behavior to PMMA at room temperature. The influence of the strain rate on the uniaxial tensile and compressive stress-strain hysteresis loops for composite A is clearly shown in figure 5.23. It is important to point out that ductility of composite A under compression is the same as the ductility of composite C.
Figure 5.20 Compressive stress-strain curves of composite A at room temperature for different strain rates until strain of 0.008

Figure 5.21 Compressive stress-strain curves of composite C at room temperature for different strain rates until strain of 0.01
Figure 5.22 Compressive stress-strain curves of composite A at displacement control rate of $5 \times 10^{-3}$ mm/s and room temperature until buckling.

Figure 5.23 Stress-strain curves of composite A for one cycle with maximum strain of 0.76% at different strain rates and room temperature.
5.3.3.2 Influence of Temperatures

Glassy (amorphous) or noncrystalline materials do not solidify in the sense as those that are crystalline. An amorphous polymer may behave like glass at low temperatures, a rubbery solid at intermediate temperatures, and a viscous liquid as the temperature is raised further. PMMA is known to have a glass transition temperature of about 100 °C. PMMA is brittle at relatively low temperature; as the temperature is raised, it becomes ductile in the vicinity of the glass transition temperatures and experiences viscoplastic yielding prior to fracture.

From the tensile experiment results at different temperatures, it was believed that the temperature has a great influence on the mechanical behavior of the acrylic particulate composite as shown in figure 5.24, figure 5.25 and figure 5.26 for composite A, composite B and composite C, respectively. At room temperature, composite A is very brittle and broken under tension long before a major strain is achieved. At the temperature over 75 °C, composite A is typical ductile material: first the peak load is reached, and then the load decreases with the increasing strain until failure. So viscoplasticity must be considered at high temperature. The interesting observation in figure 5.24 to figure 5.26 is that composite A is more ductile than composite B. Failure in composite A always happen at a larger strain than composite B for all temperatures even composite A has a higher interfacial strength than composite B.
Figure 5.24 Uniaxial stress-strain curves of composite A at different temperatures

(Celsius scale)

Figure 5.25 Uniaxial stress-strain curves of composite B at different temperatures

(Celsius scale)
5.3.3.3 Comparison between Flexural and Tensile Tests

The ultimate strength of composite A was measured using a 3-point bending test and uniaxial tensile test separately. It was found that the ultimate strength to be different at room temperature as shown in figure 5.27.
Figure 5.27 Comparison of stress-strain curve of composite A between uniaxial test and 3-point bending test at room temperature

On the plots, an apparent stress scale is indicated. For the flexure test, this stress refers to the maximum tension (or compression) stress calculated from the measured load using the relation for a uniform linear-elastic beam in bending. For the tension test the apparent stress is obtained from the measured load divided by the cross-sectional area of the test section. In both cases an initial linear elastic region is followed by nonlinear load increase to a maximum. The onset of nonlinear deflection occurred at about the same stress, 25 MPa. Although the general appearance of the stress-strain curves for flexure and tension are similar, several important details differ. The peak apparent stress is surprisingly higher in 3-point bending than in uniaxial tension (76 MPa vs. 48 MPa). These curves also differ in strains in the regions of linear load increase and nonlinear load increase. Therefore, calculation of the work done by the loading system to cause failure
(i.e., work of fracture) clearly does not give the same quantity, which is a material property independent of loading configuration.

According to Marshall (1985), in both the flexure and uniaxial tension tests, the onset of nonlinear deflection coincides with the formation of microporous zone (or crack) in the matrix. In the tension test this zone passed completely through the central test section, and the applied load was supported entirely by the binder in this zone. A large part of the additional deformation was believed to be due to the deformation of the microporous zone. The response in the flexure test was similar, except that the microporous zone penetrated only to about the midplane of the beam. The formation of the microporous zone in the matrix in only half of the flexure beam has important consequences. In particular, the micropores destroy the macroscopic uniformity of the beam and render calculation of stress based on a uniform linear elastic beam invalid. Consequently, flexural tests should not be used for the determination of ultimate strength, although it can be used for the measurement of stress and formation of a microporous zone. It is also obvious that due to the high compressive strength, assumption of linear stress distribution is not true for flexural testing.

**5.3.3.4 Influence of Interfacial Bonding Strength**

It is well known that the interfacial adhesion is an important factor influencing the tensile properties of particulate composites. Figure 5.28, figure 5.29 and figure 5.30 show the stress-strain curves of composite A, composite B and composite C at different temperatures and a constant strain rate of $1\times10^{-4}$ s$^{-1}$. It was observed that the interfacial adhesion is an important factor influencing the tensile strength of particulate composites.
It was shown that an increase in adhesive strength between the matrix and filler leads to an increase in strength at break. In contrast, weakening interface between the matrix and filler results in a reduction in strength at break. An increase in adhesive strength between the matrix and the filler below certain critical level leads to a major reduction in the ductility. Surprisingly, continuous increase in adhesive strength between the matrix and the filler will improve the ductility of the particulate composite. When the results for composite A and B are compared, we observe that A has a higher strength and is more ductile compared to B even though composite A has a higher interfacial strength. We believe this is due to the failure mechanism of the filler particles in composite A and B, which has been discussed before.

Although the tensile strength of bonded composite A is two times that of composite C at room temperature, it was observed that the debonded sample has the highest fracture toughness. Spanoudakis and Yong (1984) postulated that debonding helped crack initiation but hindered crack propagation since crack bifurcation and branching took place.
Figure 5.28 Uniaxial stress-strain curves of composite A, composite B and composite C at strain rate of $1 \times 10^{-4}$/s and room temperature

Figure 5.29 Uniaxial stress-strain curves of composite A, composite B and composite C at strain rate of $1 \times 10^{-4}$/s and 50 °C
5.3.4 Loading and Unloading Tests

Typical curves obtained from loading and unloading for composite A at a constant strain rate of $1 \times 10^{-4}$ s$^{-1}$ and various temperatures are shown in figure 5.31, figure 5.32 and figure 5.33, respectively.
Figure 5.31 Uniaxial loading and unloading test for composite A at strain rate of $1 \times 10^{-4}$/s and room temperature
Figure 5.32 Uniaxial loading and unloading tests for composite A at strain rate of $1 \times 10^{-4}/s$ and temperature 50 °C
Figure 5.33 Uniaxial loading and unloading tests for composite A at strain rate of $1 \times 10^{-4}$ /s and temperature 75 °C

Typical curves obtained from loading and unloading under strain-controlled testing for composite A at strain rate of $1 \times 10^{-4}$ and 75 °C are shown in figure 5.34. During the loading and unloading tests, the force does not return to zero upon unloading. The test specimen accumulates irreversible (residual) strain in each loading and unloading cyclic, which gradually accumulates to give gross plastic deformation. To bring the specimen to its original length will require a compressive stress to be set up.
Figure 5.34 Uniaxial loading and unloading for composite A at strain rate of $1 \times 10^{-4}$/s and temperature 75°C

Together with the damage, softening causes the reduction in strength and stiffness due to loading and unloading, which is shown clearly in figure 5.35 for the case of composite A. The area between the two curves denotes the strain energy absorbed by composite A (used to damage composite A) during the loading and unloading cycles.
After loading and unloading cycles in figure 33, then load to failure

Figure 5.35 Strength degradation of composite A due to loading and unloading at the strain rate of $1 \times 10^{-3}$/s and 75°C

5.3.5 Strain-Controlled Fatigue Tests

The maximum strain (or a measure of it) attained by particulate composites during their deformation history controls the constitutive response. Therefore, strain-controlled low fatigue tests with equal strain amplitude in tension and compression were performed. The maximum strain amplitude for the fatigue tests were selected based on the monotonic stress-strain curve obtained at room temperature. In this study, the maximum strain values corresponding to about 50%, 55%, 60%, 70%, 80% and 90% of the failure strain observed in the monotonic test were used. The constant strain rate of 0.001/s was in the fatigue tests. In all these cases, the low cycle fatigue tests were started from the zero load
and continued until the end of tests without any interruption. The data were recorded for all the cycles.

5.3.5.1 Stress-Strain Hysteresis Loops

The stress-strain hysteresis loops obtained from the uniaxial fatigue tests for composite A, composite B and composite C are shown in figures 5.36 to 5.45 at various temperatures and strain amplitudes. These curves exhibit a gradual softening (loss in stiffness) in tension due to the microscopic damage long before any visible damage occurs.

It is important to point out that little stiffness degradation was observed in the compression direction. This is probably due to the fact that, under tension, the PMMA matrix dominates the response when the fillers debond or break at an intergranular level. In the compression region cracks close and the constituents act together as a truss system in the axis of loading. In tension, load carrying capacity becomes a function of the interfacial adhesion and PMMA matrix. When complete debonding occurs, the tensile behavior is completely dominated by the PMMA matrix. In compression, there is still stress in the filler even if they are debonded. As a result, the stress-strain is not symmetric for tension and compression. Failure always occurred when the specimen was in tension. Of course it is imperative to note that the asymmetry from figure 5.36 to figure 5.44 is also a result of different strengths of the material in tension and compression.

The test specimen accumulates irreversible (residual) strain in each successive cycle, which gradually accumulates the gross plastic deformation. The phenomenon of strain softening was also observed, namely a reduction in load range with the successive
cycles. The loss in stiffness mostly occurred during the first few cycles. Moreover, the specimens also exhibited a hysteresis loop, and its area decreased with fatigue. This finding indicates that using a constant plastic strain amplitude or a constant inelastic strain energy density to model the number of cycles to failure with a Coffin-Manson type empirical equation may not yield very accurate results, yet it may lead to a reasonable first order fatigue life estimation which may be acceptable for most engineering design purposes.

![Hysteresis loops for composite A at room temperature with strain amplitude of 0.425% (fails at cycle 1270). Plot for cycle 1, 10, 100, and 1270](image)

Figure 5.36 Hysteresis loops for composite A at room temperature with strain amplitude of 0.425% (fails at cycle 1270). Plot for cycle 1, 10, 100, and 1270
Figure 5.37 Hysteresis loops for composite A at room temperature with strain amplitude of 0.6% (fails at cycle 104). Plot for cycle 1, 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, and 104

Figure 5.38 Hysteresis loops for composite A at room temperature with strain amplitude of 0.68% (fails at cycle 24)
Figure 5.39 Hysteresis loops for composite A at 50 °C with strain amplitude of 0.6% (fails at cycle 210). Plot for cycle 1, 5, 10, 20, 50, 100, 150, 180, 200, and 210.

Figure 5.40 Hysteresis loops for composite A at 75 °C with strain amplitude of 0.6% (fails at cycle 495). Plot for cycle 1, 5, 10, 20, 50, 100, 200, 300, 400, 450, 480, and 495.
Figure 5.41 Hysteresis loops for composite B at room temperature with strain amplitude of 0.6% (fails at cycle 23). Plot for cycle 1, 5, 10, 15, 20, and 23

Figure 5.42 Hysteresis loops for composite B at 50 °C with strain amplitude of 0.6% (fails at cycle 38). Plot for cycle 1, 5, 10, 15, 25, 30, 35, and 38
Figure 5.43 Hysteresis loops for composite C at room temperature with strain amplitude of 0.6% (fails at cycle 5292). Plot for cycle 1, 5, 10, 100, 500, 1000, 2000, 3000, 4000, 4500, 5000, 5100, 5200, 5250, and 5292
Figure 5.44 Hysteresis loops for composite C at 50 °C with strain amplitude of 0.6% (fails at cycle 8156). Plot for cycle 1, 5, 10, 100, 1000, 2000, 3000, 4000, 5000, 6000, 7000, 7500, 8000, 8100, and 8156

Differences among the fatigue life of the composites A, B and C demonstrate the influence of interfacial bond. Under the strain controlled fatigue tests, composite A with the strongest interfacial bond strength had the moderate fatigue life, which is a little larger than the fatigue life of composite B. Yet, composite A has a much shorter life than composite C. Average fatigue life for composite A at room temperature (among 7 samples tested) is about 104 cycles with 0.6% strain amplitude. On the other hand the average fatigue life of composite C is 8200 cycles for the same strain range and temperature. Composite B with the moderate interfacial bonding strength had the shortest fatigue life and composite C with the weakest interfacial bonding strength had the longest
Fatigue life. The difference in the fatigue life can be attributed to the difference in failure mechanisms among the 3 composites.

Debonding or cracking of the filler agglomerates diminish the resistance of the structural element. However, the matrix retains a capability to resist the extension for some time, although this occurs at a lower modulus. Only after the matrix part of the specimen has failed, one may consider that resistance has completely vanished. So the stress level in the matrix eventually determines the final fatigue life.

If we look at figures 5.28, 5.29 and 5.30, we see that composite A has a higher toughness than composite B. And toughness is defined as a measure of the ability of a material to absorb the energy up to failure. In the case of composite A with very strong bond between the matrix and the filler, the reinforcing effect is most obvious and the stress is the highest at the same strain level. This is probably due to the fact that in composite A there is a good compatibility of strain field at the interface between the filler and the matrix. As a result, the filler particles carry much higher stresses (elastic modulus of the ATH filler is 70 GPa versus 3.5 GPa elastic modulus for the PMMA matrix). When cracks initiate in the ATH particles and then proceeded to the interface and then into the matrix, the force released by the broken particles is transferred to the still intact particles and the matrix. The more the broken particles there are, the larger the stress in the matrix. When failure initiated in the interface, it was able to proceed quickly into the matrix. Eventually the stress was so high in the matrix that composite A had a relatively shorter fatigue life. Therefore, composite A has a higher toughness and longer fatigue life.

Fatigue life in the composite B was the shortest. According to the uniaxial tensile testing results, the ultimate stress level in composite B was smaller but comparable to that
in composite A. Yet, the failure strain of composite A is larger than that of composite B. Because the interfacial bonding in composite B is weaker than that in composite A, and some particles were pulled out from the matrix at certain stress levels, the total forced carried by the fillers in composite B was much smaller than that in composite A. So it is safe to assume that the stress in the matrix for composite B was larger than that in composite A. Therefore, we believe, composite A had a higher fatigue life than composite B due to difference in interfacial strength.

The tensile stress in composite A and B was much higher than that in composite C, So composite C has the longest fatigue life. Because of the debonding there were not tensile stresses in the filler, consequently the average ultimate tensile stresses was much lower and fatigue life was dominated by the ductile matrix alone. It should be pointed out that in fatigue tests even though there was a large difference between composites A, B and C in the ultimate strength in the tension region, the difference in compression region was much smaller.

Some differences were also observed between the high strain level and low strain level fatigue tests. At the very high strain levels (for example 80% or 90% of the monotonic failure strain), the stress may exceed the low strength limit of the minor weak sites inside the material. Thus, on the application of the maximum strain, a crack (or microporous zone) occurs at the weakest site that weakens the composite severely, leading to catastrophic failure in less than one hundred cycles as shown in figure 5.38. It was also obvious that the loss in stiffness mostly occurs during the first few cycles. For the low fatigue strain levels (for example 50% of monotonic failure strain), the fatigue failure in the weak site is progressive and, depending on the strain level, may span ten
thousand cycles. Some differences were also observed between different temperature fatigue tests. Softening is more prominent at elevated temperatures because of the viscosity.

5.3.5.2 Endurance Curve

In engineering practice, fatigue behavior of a material is usually characterized by a $S-N$ diagram, which shows the relationship between the strain amplitude or maximum strain and the number of cycles to failure on a semilogarithmic scale. Empirical $S-N$ curves are often utilized to predict the fatigue life. The fatigue life can be regarded either as a function of the number of cycles to failure or the time to failure. For a majority of materials, the number of cycles to failure increases continually as the strain level is reduced. Usually, the slope of the $S-N$ plot is markedly reduced at low strain level. Figure 5.45 shows the $S-N$ curves for composite A and composite B. Composite C is not included because the fatigue life of composite C is longer by almost 2 orders of magnitude than that of composite A and composite B.
Figure 5.45 $S - N$ diagram for composite A and composite B at room temperature (strain rate for the fatigue tests is 0.01/s)

Figure 5.45 indicates that even at room temperature the fatigue life of composite B and A increased significantly at a critical strain level of 0.4% and below. This strain level was the initiation of the deviation from the linear behavior in tensile stress-strain curves, as shown in the uniaxial tensile testing as shown in figure 5.18. Figure 5.45 also indicates that when the strain level was at about 0.4%, composite A and composite B had almost the same fatigue life. However at strain value of 0.6% or higher, the difference in fatigue life was significant.
5.3.5.3 Damage Measurement

The damage behavior is measured in terms of elastic modulus degradation, load-drop parameter, inelastic strain range and cumulative hysteresis dissipation, respectively.

5.3.5.3.1 Elastic Modulus Degradation

The nature of the adhesive bond at the interface between particle and matrix has a profound effect on the elastic modulus of the system. It was well recognized that there is a very good correlation between the increase in smeared crack density and the decrease in stiffness of the particulate composites. (Lemaitre, 1992; Basaran et al., 2002, 2003, 2004). Thus, crack evolution under cyclic loads can be monitored by in-situ stiffness measurements. This was framed in the theory of continuum damage mechanics with the scalar damage parameter $D$ defined as (Lemaitre, 1992):

$$D = 1 - \frac{E}{E_0}$$  \hspace{1cm} (5.1)

where $E$ is the instantaneous elastic modulus and $E_0$ is the initial value. In this project, the value of $E$ is taken as that of the average unloading modulus observed in a range of stress $0.15 \sigma_m \leq \sigma \leq 0.85 \sigma_m$ to avoid the abrupt large changes that occur at the beginning of the unloading cycles, as shown in figure 5.46.
The evolution of the damage parameter $D$ versus the number of cycles is shown in figures 5.47 to 5.50 for composite A, composite B and composite C at various temperatures and strain amplitudes.
Figure 5.47 Damage parameter $D$ as a function of number of cycles up to failure at different temperatures (in Celsius) with strain amplitude of 0.6% for composite A
Figure 5.48 Damage parameter $D$ as a function of number of cycles up to failure at room temperature with different amplitudes for composite A

Figure 5.49 Damage parameter $D$ as a function of number of cycles up to failure at different temperatures (in Celsius) with strain amplitude of 0.6% for composite B
Figure 5.50 Damage parameter $D$ as a function of number of cycles up to failure at different temperatures (in Celsius) with strain amplitude of 0.6% for composite C

Figure 5.51 Damage parameter $D$ as a function of number of cycles up to failure at room temperature with strain amplitude of 0.6% for composite A and B
It is imperative to point out that the curve slope of damage evolution versus number of cycles is independent of temperature for the range of temperatures tested in this study. Moreover, the amount of damage accumulated in the first ten cycles was more than the rest of the cycles combined. This is consistent with other experimental damage mechanics studies published in the literature, Lemaitre (1992), Zhao etc, (1999), Basaran (2003).

The slope of the damage parameter versus number of cycles was much steeper in composite B than in composite A as shown in figure 5.51. Damage evolution in composite C was very slow. This confirms the difference in fatigue life between three different types of composites used in this study. Stability of elastic modulus degradation makes it a very good parameter as a damage metric for determining degradation and the number of cycles to failure in computational damage mechanics, Tang and Basaran (2003), Basaran and Nie (2004), Basaran et al (2004).

5.3.5.3.2 Load Drop

The load-drop parameter is defined as:

\[ \varphi = 1 - \frac{\Delta \sigma}{\Delta \sigma_m} \]  

(5.2)

Where \( \Delta \sigma \) is the stress range at any cycle in the test and \( \Delta \sigma_m \) is the maximum load range which is measured in the first cycle or in the first few cycles.

Because the damaged caused by compression is negligible compared to that by tension, it is reasonable that the maximum tensile stress can be used to calculate the load-drop parameter instead of \( \Delta \sigma \) and \( \Delta \sigma_m \). Let load-drop parameter determined from
maximum tensile stress be labeled as definition 1, and load-drop parameter determined from stress range $\Delta\sigma$ be labeled as definition 2. The plots of the load-drop parameter with the number of cycles are shown in figures 5.52 to 5.57 for composite A, composite B and composite C at various temperatures.

![Graph](image)

Figure 5.52 Comparison between definition 1 and definition 2 of load-drop parameter for composite A at room temperature and strain amplitude of 0.006
Figure 5.53 Load-drop parameter (definition 1) as a function of number of cycles up to failure at different temperatures with strain amplitude of 0.6% for composite A
Figure 5.54 Load-drop parameter (definition 1) as a function of number of cycles up to failure at room temperature with strain amplitude of 0.6% for composite A

Figure 5.55 Load-drop parameter (definition 1) as a function of number of cycles up to failure at different temperatures with strain amplitude of 0.6% for composite B
Figure 5.56 Load-drop parameter (definition 1) as a function of number of cycles up to failure at different temperatures with strain amplitude of 0.6% for composite C

Figure 5.57 Load-drop parameter (definition 2) as a function of number of cycles up to failure at different temperatures with strain amplitude of 0.6% for composite C
It is interesting to note that the load drop parameter versus number of cycles to
failure curve slope is highly dependent on temperature, unlike the damage vs. number of
cycles to failure curve. Because of its simplicity and uniformity, elastic modulus
degradation is usually considered a better material degradation metric, Lemaitre (1992).

5.3.5.3.3 Plastic Strain Range

The plastic strain range is defined as $\Delta \varepsilon_p$ as shown in figure 5.58. The plots of
the plastic strain range with the number of cycles are shown in figure 5.59 to figure 5.62
for composite A, composite B and composite C at various temperatures.

![Figure 5.58 Schematic definition of plastic strain range](image-url)
Figure 5.59 Plastic strain range as a function of number of cycles up to failure at different temperatures (in Celsius) with strain amplitude of 0.6% for composite A.
Figure 5.60 Load-drop parameter as a function of number of cycles up to failure at room temperature with different amplitudes for composite A

Figure 5.61 Plastic strain range as a function of number of cycles up to failure at different temperatures (in Celsius) with strain amplitude of 0.6% for composite B
Figure 5.62 Plastic strain range as a function of number of cycles up to failure at different temperatures (in Celsius) with strain amplitude of 0.6% for composite C

Plastic strain range vs. number of cycles is also dependent on temperature, albeit not as strong as the load drop parameter. Plastic strain range experienced in each cycle does not stay constant from cycle to cycle; it gradually increases for composite C but the increase is very small for composite A and B. Especially for A, the increase is barely noticeable at room temperature, which indicates that due to very strong interfacial bond the composite is controlled by the elastic brittle filler particles. Much less so in the case of composite B. For composite C, material is able to dissipate more plastic energy as the number of cycles increase, because the response is mainly controlled by the ductile matrix.
5.3.5.3.4 Hysteresis Dissipation

The area of the hysteresis loop represents the energy dissipation corresponding to one load cycle. With each load cycle, the material absorbs a certain amount of hysteresis dissipation by which the fatigue damage may be characterized. This means that with the increasing number of cycles, the fatigue damage accumulates, corresponding to the hysteresis dissipation dissipated, until it reaches a certain critical value at which fatigue failure occurs. The plots of the hysteresis dissipation for each cycle with the number of cycles are shown in figure 5.63 to figure 5.66 for composite A, composite B and composite C at various temperatures.

Figure 5.63 Hysteresis dissipation as a function of number of cycles up to failure at different temperatures (in Celsius) with strain amplitude of 0.6% for composite A
Figure 5.64 Hysteresis dissipation as a function of number of cycles up to failure at room temperature with different amplitudes for composite A.

Figure 5.65 Hysteresis dissipation as a function of number of cycles up to failure at different temperatures (in Celsius) with strain amplitude of 0.6% for composite B.
Figure 5.66 Hysteresis dissipation as a function of number of cycles up to failure at different temperatures (in Celsius) with strain amplitude of 0.6% for composite C.

The total cumulative dissipated energy with the number of cycles is also shown in figure 5.67 for composite A at room temperature.
Figure 5.67 Cumulative hysteresis dissipation as a function of number of cycles up to failure at various temperatures (in Celsius) with strain amplitude of 0.6% for composite A

It is important to note that, when rupture is reached, damage parameter $D$, or load drop parameter $\phi$ is never equal to 1, and $D$ or $\phi$ take different values according to the intensity of the maximum strain imposed and the temperature. After a crack initiates, the failure is fast, but the elastic modulus value for the remaining intact portion of the specimen is not zero. Considering the experimental evolution of the damage parameter $D$ and $\phi$ for the acrylic casting dispersion subjected to cyclic tension-compression strain, two phases can be distinguished.

- The first phase is featured by a fast growth of damage up to about 10% of the ultimate life.
- In the second phase, damage tends to stabilize and grow very slowly until failure. This phase consists of the 90% of the fatigue life.
5.3.6 Thermal Cycling Tests

Thermal fatigue testing was also performed for composite A. The testing specimen shown in figure 5.2 was put into a thermal chamber and was fixed at the both ends using the MTS machine type 858 table top system. At the same time, temperature in the chamber was programmed to change as shown in figure 5.68. The testing data such as force, strain and time was collected by a computer. The stress-strain response for the first 3 cycles is shown in figure 5.69. It was shown that the viscoplasticity couldn’t be ignored for its thermal fatigue simulation.

![Figure 5.68 Temperature profile for the thermal fatigue tests](image)

Figure 5.68 Temperature profile for the thermal fatigue tests
Figure 5.69 First 3-cycle stress-strain responses for composite A under the thermal fatigue test

5.3.7 Creep Tests

A serious challenge when designing products to be made from polymeric materials is the prediction of performance over long periods of time, namely the creep. The amount of deformation after short or long term loading has to be known reasonably accurately in advance.

Creep phenomena are particularly common in polymers. Creep occurs when a force is continuously applied on a component, causing it to deform gradually. For polymers, the delayed response of polymer chains during deformations is the cause of creep behavior. Deformation stops when the initially folded chains reach a new equilibrium configuration (i.e. slightly stretched). Part of this deformation is recoverable after the load is removed, but recovery takes place slowly with the chains retracting by folding back to their initial state. The rate at which polymers creep depends not only on
the load, but also on temperature. In general, a loaded component creeps faster at higher temperatures.

In this section, the creep properties of acrylic composite of PMMA/ATH are determined experimentally through traditional mechanical tests, and the observed characteristics of creep are presented. The underlying deformation mechanisms, creep testing and the short time creep responses are also discussed. In standard uniaxial creep tests, the creep stress is constant and is defined as the applied load divided by the initial test specimen area. Mathematically and experimentally, the creep strain is defined as the difference between the total measured strain and the calculated elastic strain.

The details of how a creep test is performed can influence the response considerably. The initial stress rate has an impact on the creep response observed. Thus it is necessary to specify and control both the creep stress and initial stress rate in creep experiments. Great care is taken to reduce the experimental errors which can arise from poor specimen alignment, thermal distortion of the strain extensometer arms, nonuniform heating of the test specimen, and variation in the initial loading rate.

In this work, the load rate of 0.5 kN/s is used. At $T = 22^\circ C$, the ultimate tensile load for the test specimen is about 4.0 kN. Creep tests under the force of 3.6 kN (90% of ultimate tensile load), 3.2 kN (80% of ultimate tensile load), 2.4 kN (60% of ultimate tensile load), 1.6 kN (40% of ultimate tensile load) and 0.8 kN (20% of ultimate tensile load) are performed in tension. Creep tests under the force of 3.2 kN (80% of ultimate tensile load) are also performed in compression. At $T = 50^\circ C$, the ultimate tensile load for the test specimen is about 3.5 kN. Creep tests under the force of 2.8 kN (80% of ultimate tensile load), 2.1 kN (60% of ultimate tensile load), 1.4 kN (40% of ultimate tensile load), and 0.8 kN (20% of ultimate tensile load) are also performed in compression.
tensile load), and 0.7 kN (20% of ultimate tensile load) are performed in tension. At $T = 75^\circ C$, the ultimate tensile load for the test specimen is 2.5 kN. Creep tests under the force of 2.2 kN (88% of ultimate tensile load); 2.0 kN (80%), 1.5 kN (60%), 1.0 kN (40%), 0.5 kN (20%) and 0.25 kN (10%) are performed in tension. Creep tests under the force of 2.2 kN (88% of ultimate tensile load) are also performed in compression.

The most common representation of the creep data is the plot of creep strain as a function of time, where each curve represents the creep strain response for constant values of temperature and stress. The variation of total strain as a function of time with different loads is given in figure 5.70, figure 5.71 and figure 5.72 at the temperature of 22 °C, 50 °C and 75 °C, respectively. The variation of creep strain as a function of time with different loads is given in figure 5.73, figure 5.74 and figure 5.75 at the temperature of 22 °C, 50 °C and 75 °C, respectively. The variation of creep strain rate as a function of time with different loads is given in figure 5.76 and figure 5.77 at the temperature of 22 °C and 75 °C, respectively. Here the creep strain and creep strain rate is measured in terms of microstrain and microstrain per second, respectively.
Figure 5.70 Total strain as a function of time for composite A with various tensile loads at 22 °C as plotted on (A) logarithmic and (B) linear time scales
Figure 5.71 Total strain as a function of time for composite A with various tensile loads at 50 °C as plotted on (A) logarithmic and (B) linear time scales.
Figure 5.72 Total strain as a function of time for composite A with various tensile loads at 75 °C as plotted on (A) logarithmic and (B) linear time scales.
Figure 5.73 Creep strain as a function of time for composite A with various tensile loads at 22 °C as plotted on (A) logarithmic and (B) linear time scales.
Figure 5.74 Creep strain as a function of time for composite A with various tensile loads at 50 °C as plotted on (A) logarithmic and (B) linear time scales
Figure 5.75 Creep strain as a function of time for composite A with various tensile loads at 75 °C as plotted on (A) logarithmic and (B) linear time scales
Figure 5.76 Creep strain rate as a function of time for composite A with various tensile loads at 22 °C as plotted on (A) logarithmic and (B) linear time scales
Figure 5.77 Creep strain rate as a function of time for composite A with various tensile loads at 75 °C as plotted on (A) logarithmic and (B) linear time scales.
As shown in figure 5.76 and figure 5.77, the initial creep rate can be relatively high. Then the creep strain rate decreases to a relatively steady (minimum) value for a prolonged period of time. Eventually, the creep rate increases from the steady-state value and unrestrained flow occurs, leading to rupture. The primary, secondary (steady state), and tertiary creep rates and the time to rupture are strong functions of the creep stress and temperature. Increasing stress and temperature increases the creep rate and reduces the time to rupture.

The creep strength and rupture strength are frequently reported engineering data. Creep strength is the stress that produces the minimum creep rate at a specified temperature. If the frequently quoted for creep rate of $1 \times 10^{-6}$ sec$^{-1}$ is used, the creep strength of composite A at 75 $^\circ$C is about 19 MPa as shown in figure 5.78. The creep strength can also be defined as the stress to produce a specified creep strain for a specified time and temperature. The rupture strength is the stress that produces rupture at a fixed temperature in a reference period of time typically 1000, 10000 or 100000 hr.

The increase in primary creep strain with temperature for several temperatures at the stress of 25 MPa is shown in figure 5.79.
Figure 5.78 Effects of stress on the stationary creep strain rate of composite A at 75 °C as plotted on (a) logarithmic and (b) linear stationary creep strain rate scales.
Figure 5.79 Effects of temperature on the creep strain of composite A at stress of 25 MPa as plotted on (A) logarithmic and (B) linear time scales.
Plots for the creep strain and creep strain rate in both tension and compression for composite A at 22 °C are shown in figure 5.80 and figure 5.81. Although the creep strain in tension is greater than that in compression, creep rates are almost same in tension and compression at $T = 22^\circ C$. Moreover, the stationary creep strain rate is very small, so composite A can be regarded rate-insensitive material at room temperature.
Figure 5.80 Creep strain in tension and compression for composite A at 22 °C as plotted on (A) logarithmic and (B) linear time scales.
Figure 5.81 Creep strain rate in tension and compression for composite A at 22 °C as plotted on (A) logarithmic and (B) linear creep strain rate scales.
Creep rates are very different in tension and compression at \( T = 75^\circ C \). The short-time creep response is shown in figure 5.82 and figure 5.83 for several values of the stress. The results show that for nearly the same magnitude of stress in tension and compression, the magnitude of the creep rate in tension is much greater than that in compression. This difference is due partially to the fact that the creep tests are constant-load, not constant-stress tests. The creep stress is defined as the constant load divided by the initial specimen area. Therefore, in a tensile test the true stress increases as the specimen area decreases, and in compression the true stress decreases as the specimen area increases as a result of Poisson ratio effects. The most important reason for different response in tension and compression is that distanglement of molecular chains is the dominant deformation mechanism of PMMA. Tensile stresses expand the chains and reduce the resistance to distanglement, whereas compressive stresses reduce the chain dimensions and increase the resistance for distanglement.
Figure 5.82 Creep strain in tension and compression for composite A at 75 °C as plotted on (A) logarithmic and (B) linear time scales
Figure 5.83 Creep strain rate in tension and compression for composite A at 75 °C as plotted on (A) logarithmic and (B) linear creep strain rate scales.
5.4 Thermomechanical Testing of a Composite Plate with a cutout

5.4.1 Introduction

This section will provide detailed process for measuring the strain at the critical regions of a plate with cutout using strain gages. The plate is made of composite A. The following testing procedures were prepared according to the materials provided by Vishay Micro-measurements.

Despite the broad range of materials to which the strain gage has been applied (with sometimes questionable credibility), it should be recognized that the majority of practical industrial applications have been on the common structural metals, particularly steel and aluminum alloys. As a result, contemporary expertise in strain gage technology lies primarily in this segment of the materials spectrum. Composite A has radically different mechanical, thermal, and chemical properties. As a result, some of the extraneous effects which are ordinarily negligible in strain measurement on metals can become significant error sources with composite A. The properties of composite A must therefore be recognized and accounted for in each stage of the strain measurement process if accurate data are to be obtained. In addition, determination of stresses from measured strains may require the application of much more sophisticated theoretical mechanics (due to creep, etc.) than those typically employed in metals.

In terms of experimental stress analysis, one of the more significant differences between composite A and metals is in the basic mechanical properties such as the modulus of elasticity. Elastic moduli for composite A are two orders of magnitude lower than those for metals. A practical consequence of this difference is that the presence of
the installed strain gage may, at least locally, reinforce the test material. Perhaps indicative of the state of the art in strain measurement on low-modulus materials is the dearth of published data on reinforcement effects. There are indications, nevertheless, that reinforcement by the gage can lead to very large measurement errors, particularly for the lower-modulus materials.

The mechanical properties of composite A also differ noticeably from those of metals in other important respects. An example is the variation of elastic modulus with temperature. Generalization of this effect is very difficult, since it depends on the basic molecular structure, the degree of cross-linking, and the presence of copolymers; but mechanical properties can change drastically as the temperature approaches the glass-transition region. Another significant difference is in the time-dependence of the properties, as manifested in creep, stress relaxation, and sensitivity to loading rate. Obviously, these characteristics must be taken into account during the strain-measurement process, and in subsequent reduction of the data for determining stress magnitudes.

In addition to the mechanical properties of composite A, their thermal properties generally require special consideration. The thermal coefficients of expansion of composite A, for instance, are characteristically from 5 to 10 times greater than those for the structural metals. Although this need not be a factor in isothermal testing, correction or compensation for the thermal output of the strain gage can become a serious problem if measurements must be made in a variable thermal environment. Another important difference in thermal properties between composite A and the metals is in thermal conductivity. The thermal conductivity is 1 to 2 orders of magnitude lower than that of
structural metals. This property obviously affects selection of the gage size and resistance, as well as the excitation voltage, if stable gage operation is to be achieved. Gage installation technique may also be affected, since preattached leadwires are generally preferable with these materials. Additionally, the low thermal conductivity tends to compound the usual difficulty in maintaining an active and dummy strain gage continually at the same temperature in a variable thermal environment.

With metals, except for the more exotic alloys, the chemical properties of the test material do not enter significantly into the process of strain measurement. For composite A, on the other hand, the situation is often greatly different. To begin with, care must always be taken to avoid reactions between composite A and the various chemicals contained in the usual cleaning solvents, adhesives, and protective coatings. Aside from the foregoing, there can sometimes be rather severe problems in achieving or maintaining an adequate bond between the strain gage and composite A.

5.4.2 Gage Selection and Installation Procedures

Because composite A has radically different mechanical, thermal, and chemical properties from the metals, when planning to make strain gage measurements on such composites, the stress analyst should first turn to the recommendations of the gage manufacturer - not only for gage type and adhesive, but also for preferred installation procedures such as surface preparation, bonding, wiring, and environmental protection.
5.4.2.1 Gage Selection

Very short gage lengths should be avoided in order to minimize heat dissipation problems caused by the low thermal conductivity of Composite A. The specimen except the fillet is quite large but maybe severe strain gradients. Therefore, a 0.125-in (3.18-mm) gage length is specified because of the widest selection of gage patterns in this length. A gage length that is small with respect to the fillet radius (0.19-in) should also be specified for this test. A length of 0.031 in (0.8-mm) is preferable.

In the cross-section of the specimen, the directions of the principal axes are known, and single-grid gages can be employed. Of the patterns available in the selected gage length, the 125AC and 031CE pattern is a good compromise because of its high grid resistance that will help minimize heat dissipation problems. In surfaces of the specimen, the directions of the principal axes are not known, and a three-element rosette will be required. For this purpose, a planar rosette should be selected. Because of its high-resistance grid, the 125RD pattern is a good choice.

The polyimide (E) backing is preferred because its low elastic modulus will minimize reinforcement of Composite A. The normal choice of grid alloy for static strain measurement at moderate temperature is the A alloy, so the EA Series should be selected for this application.

Excessive heat application to the test model during leadwire attachment could damage the material. Option L is therefore selected so that the instrument cable can be attached directly to the leads without the application of a soldering iron to the gage proper.
In this case, the resistance was determined in the second step when the higher resistance alternative was selected from among the gage patterns. The selected gage resistance is 350 ohms.

Ideally, the gages should be self-temperature-compensated to match the model material, but this is not always feasible. In addition, the high STC gages are not typically stocked as there is not much demand for them. The best offer is similar gages from stock with more common STC values. We can use a compensating gage on an unconstrained sample subjected to the same temperature changes and subtract the output of the compensating gage from the test sample gage. The StrainSmart system can do this. Since Composite A varies widely in thermal expansion coefficient \((18\times10^{-6}/\text{F}-28\times10^{-6}/\text{F})\) from room temperature to 90 \(^0\text{C}\), STC-13 is selected.

Finally, the strain gages to be used are:

- EA-13-031CE-350/Option L (single-grid)
- EA-13-125AC-350/Option L (single-grid)
- EA-13-125RD-350/Option L (rosette)

### 5.4.2.2 Gage Installation

There can sometimes be rather severe problems in achieving an adequate bond between the strain gage and the plastic composite, especially for the "waxy" matrix such as polyethylene and polypropylene. Micro-Measurements does not maintain a database of which adhesive specifically works or doesn't work with which plastic composite.

Engineers from Micro-Measurements successfully bonded strain gages to composite A using both M-Bond 200 Adhesive and M-Bond AE-10 Adhesive at room
temperature. Neither of these adhesives attacked composite A and will be okay to use for strain measurements on composite A. But AE-10 is a must at the temperature up to 90 °C during the test.

5.4.2.2.1 Surface Preparation

Start the surface preparation by washing hands with soap and water. Also clean the work surface with M-Prep Neutralizer 5A from Vishay before beginning surface preparation.

Step 1: Degreasing

Wipe with a gauze sponge saturated with a liberal amount of isopropyl alcohol until the sponge comes up clean.

Step 2: Abrading

Flood the surface with Neutralizer 5A and lightly abrade with 400-grit silicon carbide paper. Just enough abrasive to lightly roughen the surface. Wipe dry in one direction with a clean gauze sponge. Wipe away from the gage area with a refolded or fresh sponge.

Step 3: Burnishing

With a clean straight edge and a 4H pencil, firmly burnish a layout line. Hold the pencil perpendicular to the surface.

Step 4: Conditioning

Use a liberal amount of M-Prep Conditioner A to remove all graphite from the burnished layout line by scrubbing along the line with a cotton-tipped applicator until the tip comes up clean. Then, flood and reclean the entire gaging area. Replace the
applicators when they become soiled. Next, beginning at the edge, wipe dry with gauze sponge. Refold, and dry the remaining area.

Step 5: Neutralizing

Flood the entire gage area and scrub with applicators thoroughly. Wipe dry with a clean gauze sponge.

5.4.2.2.2 Gage Bonding

Gage bonding starts by cleaning the work surface and tweezers with M-Prep Neutralizer 5A. Carefully remove the folder containing the gage from the plastic pouch. Hold it open in butterfly fashion, and grasp the gage carefully at one corner, without touching the grid. Place the gage on the clean work surface with the bonding side down.

Step 1: Gage Transfer

Use a 6-inch length of cellophane tape to transfer the gage. Center the tape over the gage and terminal assembly, then press one end to the work surface. Hold the tape at a shallow angle while smoothing it onto the gage, terminals, and work surface. Lifting the tape at a shallow angle to prevent stretching the unbonded gage, remove it from the work surface. Hold the gage with the alignment triangles over the burnished layout mark on the specimen. Press one end of the tape to the specimen and then smooth the tape, gage, and terminals into position.

Step 2: Adhesive AE-10 Mixing

Fill a clean pipette with curing agent to the line marked 10. Carefully dispense the curing agent into the center of the resin mass. Discard the pipette and immediately recap the curing agent. Vigorously stir the mixture for five minutes with a clean stirring rod.
Hold the jar near the top to prevent transfer of heat to the mixture. This will assure maximum pot life. If a room temperature cure is planned, let the mixed adhesive stand five minutes before application.

Step 3: Gage Bonding

Starting at the end away from the terminals, lift the tape at a shallow angle and form a loop exposing the bonding side of the gage and terminals. Press the free end of the tape to the specimen surface. Wipe the stirring rod clean of all liquid with a gauze sponge. Dip the clean rod into the center of the adhesive. Spread a thin layer of adhesive on the gage, the terminals, and on the specimen. Fold a gauze sponge into quarters and release the end of the tape. Hold the tape with light tension at a shallow angle to the specimen. With the folded sponge, smooth the tape onto the specimen surface. Place a silicone rubber pad on the cellophane tape directly over the gage and the terminal assembly. To distribute the clamping force evenly, center the metal backup plate over the pad.

Step 4: Tape Removal

Remove the clamp, backup plate, and silicone rubber pad from the cured installation. Peel the tape back on itself. It will peel more easily if the specimen is warm to the touch. Place a short piece of paper drafting tape over the exposed gage grid for protection.

Finally we attach leadwires to strain gages and coatings them against moisture and other contaminants that might affect gage stability. Both encapsulated and open-faced gages, and their leadwire connections, must be protected.
5.4.3 Correction and Compensation

When strain measurements are completed, it is often necessary to adjust the data for known and correctable errors prior to data reduction for principal strains and stresses. At small strain conditions, typical corrections include those for transverse sensitivity, thermal output, and gage factor variation with temperature. Thermal output is potentially the most serious error source in the practice of static strain measurement with strain gages. When the Poisson's ratio differs significantly from 0.29, correction for the transverse sensitivity of strain gages is generally necessary.

In theory, the error due to thermal output can be completely eliminated. One option is to select a gage type with the nearest STC number and then calibrate the gage/test-material combination for its thermal output over the specified temperature range. Subsequently, if gage temperature is measured along with the strain, the indicated strain data can be corrected for the thermal output. An alternative is to employ, in conjunction with the "active" strain gage, but connected in an adjacent arm of the Wheatstone bridge circuit, an identical compensating or "dummy" gage - mounted on an unstrained specimen made from the identical material as the test part, and subjected always to the same temperature as the active gage as shown in figure 5.84. Under these hypothetical conditions, the thermal outputs of the two gages should be identical. And, since identical resistance changes in adjacent arms of the Wheatstone bridge do not unbalance the circuit, the thermal outputs of the active and dummy strain gages should cancel exactly - leaving only the stress-induced strain in the active strain gage to be registered by the strain indicator. The dummy and active gages should have the same STC number, and should be taken from the same manufacturing lot to minimize differences in thermal
output characteristics. For this to be precisely true, the leadwires to the active and dummy gages should be of the same length and be routed together so that their temperature-induced resistance changes also match identically. In general, when the three identity criteria already mentioned can be well satisfied, the method of compensating with a dummy gage is a very effective technique for controlling the thermal output error.

![Diagram of Wheatstone bridge and strain gages](image)

Figure 5.84 Examples illustrating the use of a second (compensating) strain gage in an adjacent Wheatstone bridge arm to cancel the effect of thermal output

The principal problems encountered in this method of temperature compensation are those of establishing and maintaining the three sets of identical conditions postulated above. To begin with, it is sometimes very difficult to arrange for the placement of an unstrained specimen of the test material in the test environment; and even more difficult to make certain that the specimen remains unstrained under all test conditions. There is a further difficulty in ensuring that the temperature of the compensating gage on the unstrained specimen is always identical to the temperature of the active gage. This problem becomes particularly severe whenever there are temperature gradients or transients in the test environment. And, the same considerations apply to the leadwires. Finally, it must be recognized that no two strain gages - even from the same lot or
package - are precisely identical. For most static strain measurement tasks in the general neighborhood of room temperature, the difference in thermal output between two gages of the same type from the same lot is negligible; but the difference may become evident (and significant) when measuring strains at temperature extremes such as those involved in high-temperature or cryogenic work. In these instances, point-by-point correction for thermal output will usually be necessary. With non-self-temperature-compensated gages, the gage-to-gage differences in thermal output may be so great as to preclude dummy compensation for temperatures which are remote from room temperature. We will use the first approach to cancel the thermal output in the test.

Errors in strain indication due to transverse sensitivity are generally quite small since the transverse sensitivity itself is small. However, in biaxial strain fields characterized by extreme ratios between principal strains, the percentage error in the smaller strain can be very great if not corrected for transverse sensitivity. On the other hand, in the particular case of uniaxial stress in a material with a Poisson's ratio of 0.285, the error is zero because the gage factor given by the manufacturer was measured in such a uniaxial stress field and already includes the effect of the Poisson strain. It is important to note that when a strain gage is used under any conditions other than those employed in the gage-factor calibration, there is always some degree of error due to transverse sensitivity. In other words, any gage which is: (a) installed on a material with a different Poisson's ratio of 0.285; or (b) installed on steel, but subjected to other than a uniaxial stress state; or (c) even installed on steel with a uniaxial stress state, but aligned with other than the maximum principal stress, exhibits a transverse-sensitivity error which may require correction.
The error due to transverse sensitivity for a strain gage oriented at any angle, in any strain field, on any material, can be expressed as:

\[ e = \frac{K_i \left( \frac{\varepsilon_t}{\varepsilon_a} + \nu_0 \right)}{1 - \nu_0 K_i} \times 100 \]  

(5.3)

where:

- \( K_i \) is the transverse sensitivity coefficient
- \( e \) = the error as a percentage of the actual strain along the gage axis.
- \( \nu_0 \) = the Poisson's ratio of the material on which the manufacturer's gage factor, was measured (usually 0.285)
- \( \varepsilon_a, \varepsilon_t \) = respectively, the actual strains parallel and perpendicular to the primary sensing axis of the gage.

The effects of transverse sensitivity should always be considered in the experimental stress analysis of a biaxial stress field with strain gages. Since a three-gage rosette will be used in the test, simple correction methods are given here for the three-gage rectangular rosette. Unless otherwise noted, these corrections apply to rosettes in which the transverse sensitivities of the individual gage elements in the rosettes are equal to one another, or approximately so. Correction for the effects of transverse sensitivity can be made either on the individual strain readings or on the principal strains or principal stresses calculated from these. Numbering the gage elements consecutively, the correction equations for all three gages are listed:

\[ \varepsilon_1 = \frac{1 - \nu_0 K_i}{1 - K_i^2} \left( \hat{\varepsilon}_1 - K_i \hat{\varepsilon}_3 \right) \]  

(5.4)
\[ \varepsilon_1 = \frac{1 - \nu_0 K_i}{1 - K_i^2} \left[ \hat{\varepsilon}_2 - K_i \left( \hat{\varepsilon}_1 + \hat{\varepsilon}_3 - \hat{\varepsilon}_2 \right) \right] \]  

(5.5)

\[ \varepsilon_3 = \frac{1 - \nu_0 K_i}{1 - K_i^2} \left( \hat{\varepsilon}_3 - K_i \hat{\varepsilon}_1 \right) \]  

(5.6)

where:

\( \hat{\varepsilon}_1, \hat{\varepsilon}_2, \hat{\varepsilon}_3 \) = indicated strains from the respective gage elements.

\( \varepsilon_1, \varepsilon_2, \varepsilon_3 \) = corrected strains along the gage axes.

5.4.4 Determination of Stresses

Determination of stresses from measured strains requires the application of much more sophisticated theoretical mechanics. An example is the variation of the elastic modulus with temperature. In addition, composite A is nonlinear in its stress/strain behavior. One of the most significant factors is in the time-dependence of the properties at high temperature, as manifested in creep, stress relaxation, and sensitivity to loading rate. These characteristics must be taken into account during the strain-measurement process, and in subsequent reduction of the data for determining stress magnitudes.

5.4.5 Test Setup

The plate dimension, distribution of temperature control points and strain gage points are shown in figure 5.85, figure 5.86 and figure 5.87, respectively.
Figure 5.85 Dimension of the composite plate with a cutout (mm)

Figure 5.86 Distribution of the temperature control points (mm)
The heating process is controlled by the thermal couple at the control points. The plate is first uniformly heated for 10 minutes until the temperature at the control points reaches 90 °C. Then the temperature at the control points is kept at 90 °C for another 10 minutes. Finally the plate is cooled down to room temperature by a fan located under the center of plate for 100 minutes. The temperature profile for the temperature control points is shown in figure 5.88. The heating and cooling units are controlled through an Integral gain, Derivative gain, Feed forward gain and Stabilization gain (PIDF) tuning controller.
The Vishay micro-measurements system 5000 is used for measuring the strain in the test. This system utilizes StrainSmart software interfaced through a digital communications link to instrumentation hardware for stress analysis testing under a wide variety of conditions. The StrainSmart software allows straightforward configuration and is designed for ease-of-use in collecting strain gage data.

In order to eliminate the error due to thermal output, thermal output over the specified temperature range must be calibrated from the gage/composite combination. In this project, the thermal output was measured when the gage/plate assembly was heated at rate of 100°C per hour. The plate is 1.5 mm in thickness for the achievement of uniform temperature distribution over thickness. At the same time, the gage temperature is measured along with the strain measurement. The testing system is shown in figure 5.89, figure 5.90, figure 5.91 and figure 5.92.

Figure 5.88 Temperature profile at the temperature control points
Figure 5.89 USB temperature data acquisition system

Figure 5.90 Thermal plate used to heat strain gage/composite assembly

Figure 5.91 Thermal output measurement system
5.4.6 Test Results

5.4.6.1 Thermal Output

In order to eliminate creep effects in the adhesive AE10, the strain gage/composite assembly is postcured at the temperature of 105 °C for 12 hours. The thermal output for the strain gage EA-13-125AC-350, strain gage EA-13-031DE-350 and strain gage EA-13-125RD-350 are shown in figure 5.92, figure 5.93 and figure 5.94, respectively. Strain gage EA-13-125AC-350, EA-13-031DE-350 and EA-13-125RD-350 work very well up to 95 C.

![Graph showing thermal strain as a function of temperature](image)

Figure 5.92 Thermal strain as a function of temperature for strain gage EA-13-125AC-350/composite assembly
Figure 5.93 Thermal strain as a function of temperature for strain gage EA-13-031DE-350/composite assembly

Figure 5.94 Thermal strain as a function of temperature for strain gage EA-13-125RD-350/composite assembly
5.4.6.2 Thermal Cycling Tests of Composite Plates

The locations of strain gages are shown in figure 5.95. Strain gage a, strain gage e, strain gage e' and strain gage e'' are along the middle thickness of the plate. Strain gage b and strain gage b' are on the top surface of the plate and strain gage c is on the bottom surface. Strain gage d is at the one third of thickness close to top surface, and strain gage f is at the one third of the thickness close to bottom surface. Furthermore, strain gage b and strain gage b' are symmetric about the center line of plate. Strain gage e and strain gage e' are also symmetric about the center line of plate. Strain gage e'' measures the strain in z’ direction, Strain gage a, strain gage d, strain gage e, strain gage e’, and strain gage f measure the strain in x’ direction. Strain gage b, strain gage b’, and strain gage c measure the strain in x’ and y’ direction. The principal strains $\varepsilon_1$ and $\varepsilon_2$ for them were plotted.

Figure 5.95 Strain gage locations
The strain in *strain gage a* is shown in figure 5.96, which is very small. The maximum and minimum strain for *strain gage b* and *strain gage b'* are shown in figure 5.97, figure 5.98, figure 5.99 and figure 5.100, respectively. Because *strain gage b* and *strain gage b'* are symmetric about the center of plate, the measured results are almost the same. It is expected that there is a temperature gradient over the thickness of the plate. The comparison of strain on the top surface with that on bottom is shown in figure 5.101, figure 5.102, figure 5.103 and figure 5.104. The strains in the corners of cutout, including strain in both thickness and plane direction, are shown in figure 5.105, figure 5.106, figure 5.107 and figure 5.108.

![Figure 5.96 Strain in strain gage a as a function of time for test #2](image)

Figure 5.96 Strain in *strain gage a* as a function of time for test #2
Figure 5.97 Maximum strain in strain gage b as a function of time for test #2

Figure 5.98 Minimum strain in strain gage b as a function of time for test #2
Figure 5.99 Maximum strain in strain gage b' as a function of time for test #2

Figure 5.100 Minimum strain in strain gage b' as a function of time for test #2
Figure 5.101 Maximum strain in strain gage b as a function of time for test #3

Figure 5.102 Minimum strain in strain gage b as a function of time for test #3
Figure 5.103 Maximum strain in strain gage $c$ as a function of time for test #3

Figure 5.104 Minimum strain in strain gage $c$ as a function of time for test #3
Figure 5.105 Strain in *strain gage d* as a function of time for test #3

Figure 5.106 Strain for *strain gage f* as a function of time with test #3
Based upon the test results, the strain at the corner in x direction is largest in magnitude. The cracks always occur first at the corner of cutout during the cooling time,
and then spread with the cycles during the experiments. The cracks destroy the strain gage, which led to the loss of the strain data recording. Figure 5.109 shows the strain in strain gage \( e' \) and strain gage \( e'' \) as a function of time for test #1 after cycle 21. The crack in the corner is shown in figure 5.110.

Temperature distribution in the plate is rather complicated. The temperature gradient is very large around the heating hole in both directions, namely in the plane and thickness direction. The temperature distribution in the plane is shown in figure 5.111.

Figure 5.109 Strain in strain gage \( e' \) and strain gage \( e'' \) as a function of time for test #1 after cycle 21
Figure 5.110 Cracks near the corner of cutout in the composite plate

Figure 5.111 Temperature distribution in plate around heating source when the maximum temperature of controlled points is 120 °C
CHAPTER 6

Verifications and Applications

6.1 Introduction

Commercially available general-purpose finite element analysis (FEA) codes, such as ABAQUS, ANSYS, NASTRAN, cannot directly perform thermomechanical damage analysis for acrylic particulate composites due to a lack of a unified constitutive model with damage evolution capacity. Because of the complicated material properties of acrylic particulate composites, the available viscoplastic models embedded in the commercial FEA software may not appropriately reflect the time and temperature dependent response of the acrylic particulate composite, such as the interfacial transitional zone between the filler and the matrix, the CTE mismatch between the filler and the matrix. On the other hand, the fatigue lifetime prediction is usually made based on the calculated stress, strain or strain energy, and Coffin-Manson empirical curves. The coupled effects of material degradation during fatigue are not taken into consideration by the commercial FEA codes. That is, the material properties are considered as unchanged no matter how much damage has been caused by the fatigue process during the thermomechanical cycling.

In order to predict the thermomechanical damage behavior in acrylic particulate composites, the damage coupled viscoplastic model with kinematic and isotropic hardening, developed in chapter 4 and 5, is programmed in FORTRAN codes, and implemented into ABAQUS through user-defined subroutine UMAT. Thus, the finite
element analysis procedure can be conducted, with the combination of the proposed constitutive model with the ABAQUS nonlinear numerical solver, preprocessor and postprocessor, to simulate the behavior of acrylic particulate composites under thermomechanical fatigue loading.

The behavior of acrylic particulate composites is simulated as a nonlinear static procedure with an initial boundary condition. The nonlinear procedure is solved incrementally by dividing the time interval into numbers of successive time steps. For each time step, global equilibrium equations, with specific loading, boundary conditions and defined material properties, are solved by ABAQUS with the general return mapping algorithm to obtain the strain increment. At each strain increment, along with the initial conditions determined by the last time step, the stress and internal state variables, e.g. the damage variable, are integrated and updated within user defined material subroutines at each integration point. The general return mapping algorithm is used for viscoplastic strain computations. The residual equations for each integration point of all elements are checked, and the convergence is iteratively reached at each time step.

For verification of the constitutive model and numerical procedure, computational simulations of the uniaxial monotonic tensile and fatigue tests for particulate composite A under various temperatures and strain rates were performed. The simulation results were compared with the corresponding experimental test data for validation. The effects of bonding conditions and CTE mismatch between matrix and particles were predicted under thermomechanical loading conditions. The simulated damage evolution of particulate composite A was also compared with experimentally measured elastic
modulus degradation, which is considered as one criterion of material damage under thermomechanical fatigue.

The simulation was also performed for the mechanical behavior of a plate with cutout under thermal cycling loadings. For validation, the numerical simulation results were compared with the corresponding test data from laboratory measurements using the strain gage. And finally, the thermomechanical fatigue lifetime of a plate with a cutout under thermomechanical loads was predicted using the damage metric proposed in this dissertation.

6.2 Determination of Material Parameters

In chapter 3 and chapter 4, the damage evolution function and the micromechanics based modeling for particulate composites were developed. In order to successfully simulate the damage coupled viscoplasticity of particulate composites, it is important to determine the appropriate material parameters for the model. Experimental tests that simulate in-service loading conditions are required to obtain reliable material parameters needed by the constitutive model. Due to the time and temperature dependent mechanical properties of acrylic particulate composites, it is desirable that tests are conducted under different loading rates and different temperatures. In addition, we also need to know the thermomechanical properties of the particle and the matrix, which determine the overall properties of the particulate composites.
6.2.1 Properties of ATH

In the model, ATH is regarded as an isotropic elastic material. The thermomechanical properties of ATH as provided by the sponsor were as follows:

Poisson ratio of ATH: $\nu_f = 0.24$

Elastic modulus of ATH: $E_f = 70000\text{MPa}$

Coefficient of thermal expansion of ATH: $\alpha_f = 1.47 \times 10^{-6} / {}^\circ\text{C}$

The average diameter of ATH is 35$\mu\text{m}$

6.2.2 Properties of PMMA

The matrix PMMA is a very common polymer, which has been extensively studied. The young's modulus of PMMA as function of temperature is taken from the works of Cheng et al. (1990) as shown in figure 6.1.

$$E_m = -0.0234T + 4.124 \quad \text{(GPa)} \quad (6.1)$$

where $T$ is the temperature in Celsius.
The Poisson’s ratio of PMMA provided by the sponsor was: $\nu_m = 0.31$.

The CTE of PMMA is assumed to be the same as that of the particulate composite, which will be discussed later.

### 6.2.3 Properties of Interphase

The interphase around the particle is also regarded as an isotropic elastic material. The Young’s modulus and thickness of the interphase are adjustable parameters in the proposed model. In addition, it is reasonable to assume that the Poisson ratio and CTE of the interphase are the same as that of the matrix (PMMA), however, the Young’s modulus of the interphase is less than that of PMMA. For these simulations, the thickness of the interphase is taken as 1% of the diameter of filler particles; the Young's modulus is half of that of PMMA except where specified differently.
6.2.4 Properties of Particulate Composites

The following thermomechanical properties of the particulate composite A are determined according to the data provided by the sponsor.

The average specific mass for the composite: \( m_i = 85\text{g/mole} \)

Density of the composite: \( \rho = 1750\text{Kg/m}^3 \)

Volume fraction of particle in the composite: \( \phi = 0.48 \)

The Poisson’s ratio of the composite A is given as a function of temperature as shown in figure 6.2:

\[
\nu = 0.008T + 0.334
\]  

(6.2)

![Figure 6.2 Poisson’s ratio of composite A as a function of temperature](image)

The coefficient of thermal expansion of the composite A is given as function of temperature as shown in figure 6.3:

When \( T \leq 90^\circ\text{C} \)
\[ \alpha = 3.035 \times 10^{-7} T + 2.347 \times 10^{-5} \quad (6.3a) \]

When \( T \geq 90^\circ C \)

\[ \alpha = 1.0992 \times 10^{-6} T - 5.012 \times 10^{-5} \quad (6.3b) \]

![Figure 6.3 Coefficient of thermal expansion (CTE) of composite A as a function of temperature](image)

Viscosity \( \eta \) is the ratio of the loss modulus to the angular frequency, which is determined during the forced harmonic oscillation test (Nielsen and Landel, 1994). The viscosity relaxation time \( \tau \) is defined as (Simo and Hughes, 1998)

\[ \tau = \frac{\eta}{2\mu} \quad (6.4) \]

where \( \mu \) is the shear modulus. It is important to realize that the controlling factor in the relaxation process is the relative time \( t/\tau \). The absolute time \( t \) is regarded as short or
long only when compared with $\tau$. The concept of relaxation time is explained in greater
details by Simo and Hughes (1998). According to the dynamic mechanical testing data
provided by the sponsor, the viscosity relaxation time $\tau$ is determined as shown in
figure 6.4:

When $T \leq 90^\circ C$

$$\tau = 1.12406 \times 10^{-6} T^3 - 1.67823 \times 10^{-4} T^2 + 7.91134 \times 10^{-3} T + 7.35 \times 10^{-3}$$  \hspace{1cm} (6.5a)

When $T \geq 90^\circ C$

$$\tau = -2.6348 \times 10^{-6} T^4 + 1.08452 \times 10^{-3} T^3 - 1.64629 \times 10^{-1} T^2 + 10.9673T - 271.11$$  \hspace{1cm} (6.5b)

![Figure 6.4 Relaxation time of composite A as a function of temperature](image)

The elastic modulus of composite A can be determined from the properties of the
particle, the matrix and the interphase according to the proposed micromechanical model
for particulate composites. The elastic modulus of composite A is also determined from
our uniaxial tensile tests with a different strain rate and temperature as shown in figure 6.5.

\[ E_m = -0.0005T^2 - 0.021T + 13.33 + 0.6 \log(\dot{\varepsilon}) \quad \text{(GPa)} \]  

(6.6)

![Graph showing Elastic modulus of composite A as a function of temperature](image)

Figure 6.5 Elastic modulus of composite A as a function of temperature

The gas constant is also needed for the damage evolution function, where its value is given as follows:

\[ R = 8.3145 \text{Joule/mole/K} \]

6.3 Monotonic Stress-Strain Response

Stress-strain response essentially characterizes the mechanical behavior of materials. The applicability of the numerical procedure by implementing the constitutive model developed in chapter 4 into ABAQUS was verified by the simulations of the monotonic stress-strain response of composite A at different temperatures with different
strain rates. The comparisons of the simulation results with test data were made for validation.

The geometry of the specimen used in the uniaxial tests is shown in figure 5.2. Owing to the symmetry, only one half of the gauge length was used for simulation. To simulate the strain controlled uniaxial tests, the uniform displacement was applied to the end of the bar.

It is well recognized that there is a very good correlation between the increase in crack density and the decrease in stiffness of the particulate composites. Thus, the damage evolution under loads can be monitored by *in-situ* stiffness measurements. This is framed in the theory of continuum damage mechanics with the scalar damage parameter \( D \) defined as (Kachanov, 1986):

\[
D = 1 - \frac{E}{E_0}
\]  

(6.7)

where \( E \) is the instantaneous elastic modulus and \( E_0 \) is the initial value of the elastic modulus. This damage parameter was determined experimentally and compared with the damage predicted by the proposed damage evolution function developed in chapter 3.

### 6.3.1 Isotropic Hardening Parameters

The Ramberg-Osgood isotropic hardening model is used to model the monotonic tensile yield stress, which is reasonably accurate for the uniaxial tensile behavior.

\[
\bar{\sigma}_y = \bar{\sigma}_0 + K\bar{\alpha}^n
\]  

(6.8)

where \( \bar{\sigma}_0 \) is the initial yield stress for composite A and \( \bar{\alpha} \) is the equivalent viscoplasticity, which is given by equation (4.267)
\[ \hat{\alpha} = \sqrt{\bar{T}_1 + 2\bar{T}_2} \sqrt{\bar{\varepsilon}^p : \bar{T}^{-1} : \bar{\varepsilon}^p} \]

The temperature dependent constants $K$ and $n$ for the Ramberg-Osgood isotropic hardening model can be easily determined from experimental data near the yield point, where the damage is believed to be negligible. The stress as a function of the viscoplastic strain for composite A at various temperatures is shown in figure 6.6.

![Figure 6.6 Stress as a function of viscoplastic strain for composite A at various temperatures](image)

The parameters for the Ramberg-Osgood isotropic hardening model are determined from the monotonic uniaxial tensile tests at various temperatures. The results are shown in figure 6.7, figure 6.8 and figure 6.9.

\[ \overline{\sigma}_0 = -0.1791T + 19.6 \quad T \leq 100^\circ C \quad (6.9) \]

\[ K = -8.5881 \times 10^{-4} T^3 + 9.1312 \times 10^{-2} T^2 - 4.8155 T + 424.9 \quad T \leq 100^\circ C \quad (6.10) \]
\[ n = 4.098 \times 10^{-7} T^3 - 4.476 \times 10^{-5} T^2 + 2.33 \times 10^{-3} T + 0.3542 \quad T \leq 100^\circ C \] (6.11)

where \( T \) is the temperature in Celsius.

Figure 6.7 Initial yield stress of composite A as a function of temperature

Figure 6.8 Parameter K of composite A as a function of temperature
The critical damage parameter for composite A is also determined from the uniaxial tensile tests at various temperatures as shown in figure 6.10.

\[ D_{cr} = 0.1972T + 50.22 \quad T \leq 100^\circ C \quad (6.12) \]

where \( T \) is the temperature in Celsius. \( D_{cr} \) is determined using the trial and error method by matching the damage determined from the elastic modulus degradation with the damage calculated from the internal entropy production (equation (3.81)) in the case of uniaxial tensile tests.
6.3.2 Finite Element Simulation Results

The stress-strain response obtained from the damage coupled viscoplastic model was compared with the viscoplastic model without damage and experimental data as shown in figure 6.11 and figure 6.12 at 24 °C and 75 °C, respectively. These simulation results are obtained based on the assumption that the thickness of interphase is 1% of the diameter of the particle and the elastic modulus of interphase is 50% of that of PMMA. Furthermore, the CTE mismatch effects are also included, where the temperature when residual stresses begin to build up, is assumed to be 100 °C. It is seen that the damage effects must be accounted for at relatively large strains and the proposed damage evolution function performs very well.

The comparison of the damage parameter obtained from the damage coupled plastic model with that measured in experiments in terms of elastic modulus degradation is given in figure 6.13 and figure 6.14, respectively. The simulation is in qualitative
agreement with the experimental data for engineering purposes. The comparison between the measured elastic modulus degradation and simulation results from the damage evolution function validates that entropy can be used as a criterion for fatigue lifetime prediction.

Figure 6.11 Comparison of stress-strain relationship among damage coupled viscoplastic model, viscoplastic model without damage and experiment data at 24 °C
Figure 6.12 Comparison of stress-strain relationship among damage coupled viscoplastic model, viscoplastic model and experiment data at 75 °C
Figure 6.13 Comparison of damage parameter obtained from damage model with that measured in experiments in terms of elastic modulus degradation at 24 °C.
Figure 6.14 Comparison of damage parameter obtained from damage model with that measured in experiments in terms of elastic modulus degradation at 75 °C

6.3.3 Parametric Studies

The influence of CTE mismatch between the particle and the matrix on the overall uniaxial behavior of composite A is shown in figure 6.15 and figure 6.16 at 24 °C and 75 °C, respectively. Here, $T_c$ is the temperature that the residual stresses are set up in the microstructure due to the CTE difference between PMMA and ATH as cooling the composite from its curing temperature. These simulation results are obtained based on the assumption that the thickness of the interphase is 1% of the diameter of the particle and the elastic modulus of interphase is 50% of that of PMMA. Based on the simulation
results, the CTE mismatch between the matrix and the particle has negligible influence on the overall stress-strain relationship.

Figure 6.15 Effect of the CTE mismatch between the matrix and the particle on the stress-strain relationship of composite A at 24 °C
Figure 6.16 Effect of the CTE mismatch between the matrix and the particle on the stress-strain relationship of composite A at 75°C

The influence of stiffness of the interphase around the particle on the overall uniaxial behavior of composite A is shown in figure 6.17 and figure 6.18 at 24°C and 75°C, respectively. These results are obtained by only changing the Young’s modulus of the interphase as the percent of that of the matrix and keeping other parameters fixed ($T_c = 100^\circ$C and the thickness of interphase is 1% of the diameter of particle). Based on the simulation results, the stiffness of the interphase has significant influence on the overall stress-strain relationship. Increasing the stiffness of the interphase leads to larger stiffness of the composite.
Figure 6.17 Effect of the stiffness of interphase around particle on the stress-strain relationship of composite A at 24 °C

Figure 6.18 Effect of the stiffness of interphase around particle on the stress-strain relationship of composite A at 75 °C
The influence of thickness of the interphase around the particle on the overall uniaxial behavior of composite A is shown in figure 6.19 and figure 6.20 at 24°C and 75°C, respectively. These results are obtained by only changing the thickness of the interphase as a percent of the diameter of the particle and keeping other parameters fixed ($T_c = 100°C$ and the elastic modulus of interphase is about 50% of that of PMMA). Based on the simulation results, the thickness of the interphase also has significant influence on the overall stress-strain relationship. Increasing the thickness of the interphase decreases stiffness of the composite.

![Figure 6.19 Effect of the thickness of interphase around particle on the stress-strain relationship of composite A at 24°C](image)

Figure 6.19 Effect of the thickness of interphase around particle on the stress-strain relationship of composite A at 24°C.
Figure 6.20 Effect of the thickness of interphase around particle on the stress-strain relationship of composite A at 75 °C

The influence of the yield strength of composite A on the overall uniaxial behavior of composite A is shown in figure 6.21 and figure 6.22 at 24 °C and 75 °C, respectively. These results are obtained by only changing the isotropic hardening function for composite A and keeping other parameters fixed (\(T_e = 100°C\) and the elastic modulus of interphase is about 50% of that of PMMA, thickness of interphase is 1% of the diameter the of filler). Based on the simulation results, the yield surface of the composite has significant influence on the overall stress-strain relationship. Increasing the yield stress of the composite will leads to larger ultimate strength of the composite.
Figure 6.21 Effect of the yield strength of composite A on the stress-strain relationship of composite A at 24 °C.

Figure 6.22 Effect of the yield strength of composite A on the stress-strain relationship of composite A at 75 °C.
The influence of particle volume fraction on the overall uniaxial behavior of composite A is shown in figure 6.23 and figure 6.24 at 24°C and 75°C, respectively. These results are obtained by only changing the particle volume fraction and keeping other parameters fixed ($T_c = 100°C$ and the elastic modulus of interphase is about 50% of that of PMMA, thickness of interphase is 1% of diameter of filler). Based on the simulation results, the particle volume fraction has significant influence on the overall stress-strain relationship. Increasing the particle volume fraction leads to larger stiffness of the composite.

Figure 6.23 Effect of the particle volume fraction on the stress-strain relationship of composite A at 24°C
The influence of the elastic modulus of the matrix on the overall uniaxial behavior of composite A is shown in figure 6.25 and figure 6.26 at 24 °C and 75 °C, respectively. These results were obtained by only changing the elastic modulus of the matrix of composite A and keeping other parameters fixed ($T_c = 100^\circ C$ and the elastic modulus of interphase is about 50% of that of PMMA, thickness of interphase is 1% of the diameter of the filler). Based on the simulation results, the stiffness of the matrix has significant influence on the overall stress-strain relationship. Increasing the stiffness of the matrix leads to larger stiffness of the composite.
Figure 6.25 Effect of the elastic modulus of matrix on the stress-strain relationship of composite A at 24°C

Figure 6.26 Effect of the elastic modulus of matrix on the stress-strain relationship of composite A at 75°C
The influence of the elastic modulus of the particle on the overall uniaxial behavior of composite A is shown in figure 6.27 and figure 6.28 at 24 °C and 75 °C, respectively. These results are obtained by only changing the elastic modulus of the particle and keeping other parameters fixed ($T_c = 100^\circ C$ and the elastic modulus of interphase is about 50% of that of PMMA, thickness of interphase is 1% of the diameter of the filler). Based on the simulation results, the stiffness of the particle has significant influence on the overall stress-strain relationship. Increasing the stiffness of the particle leads to larger stiffness of the composite.

Figure 6.27 Effect of the elastic modulus of particle on the stress-strain relationship of composite A at 24 °C
6.4 Cyclic Stress-Strain Response

In this section, the isothermal uniaxial cyclic fatigue tests were simulated by implementing the damage coupled viscoplastic constitutive model into ABAQUS. To simulate the strain controlled uniaxial tests, the uniform displacement was applied to the end of the bar. For the fatigue test with the strain amplitude of 0.6%, the displacement profile is shown in figure 6.29.
6.4.1 Kinematic Hardening Parameters

For simplicity, the linear kinematic hardening plastic model was used to model the cycling response, which gives only the first approximation of the material behavior subjected to cyclic loading. It is very important to determine the appropriate linear kinematic hardening parameters, which are believed to be temperature and strain dependent. The initial yield stress and hardening modulus $H$ for the linear kinematic model are determined from experimental data with a strain amplitude of 0.6% at various temperatures. The initial yield stress $\sigma_0$ was assumed to be constant, and it can be easily determined from the stress-strain curves at various temperatures. For example, the initial yield stress at room temperature is determined to be about 39 MPa according to the stress-strain curves of the fatigue test with strain amplitude of 0.6% at room temperature as shown in figure 6.30.
Figure 6.30 The 1st cycle stress-strain curve in tension direction for the cyclic tests with the strain amplitude of 0.6% at room temperature.

Using the same method, the initial yield stress at various temperatures has been determined as shown in table 6.1. These data was plotted using EXCEL as shown in figure 6.31. Finally, we have the initial yield stress for the linear kinematic model as given in equation (6.13)

\[
\bar{\sigma}_0 = -0.3356T + 50.1 \quad T \leq 100^\circ C
\]  

(6.13)

Table 6.1 Initial yield stress for linear kinematic model

<table>
<thead>
<tr>
<th>Temperature (Celsius)</th>
<th>24</th>
<th>40</th>
<th>50</th>
<th>60</th>
<th>75</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yield stress (MPa)</td>
<td>39</td>
<td>34</td>
<td>30</td>
<td>27</td>
<td>22</td>
</tr>
</tbody>
</table>
The hardening modulus $H$ for the linear kinematic model was determined from experimental data with a strain amplitude of 0.6% at the beginning of the 5th cycle, which is believed to be the stabilized cycle. The 5th stress-strain curves of the fatigue test with strain amplitude at room temperature as shown in figure 6.32, from which the kinematic hardening modulus $H$ can be determined from the following equation

$$H = \frac{\Delta \sigma}{\Delta e^{\gamma}}$$  \hspace{1cm} (6.14)

where $\Delta \sigma$ is the stress increment beyond yield stress for any strain increment; $\Delta e^{\gamma}$ is the inelastic strain corresponding to $\Delta \sigma$.

According to figure 6.32 and equation (6.14), the kinematic hardening modulus at room temperature was calculated to be about 32000 MPa. Using the same method, the kinematic hardening modulus at various temperatures has been determined as shown in

---

Figure 6.31 Initial yield stress of composite A for the linear kinematic model as a function of temperature
table 6.2. These data was plot using EXCEL as shown in figure 6.33. Finally we have the kinematic hardening modulus for the linear kinematic model as given in equation (6.15)

\[ H = 1.9868T^2 - 597.15T + 45914 \quad T \leq 100^\circ C \quad (6.15) \]

Table 6.2 Kinematic hardening modulus for linear kinematic model

<table>
<thead>
<tr>
<th>Temperature (Celsius)</th>
<th>24</th>
<th>40</th>
<th>50</th>
<th>60</th>
<th>75</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yield stress (MPa)</td>
<td>32000</td>
<td>23500</td>
<td>20000</td>
<td>17000</td>
<td>11000</td>
</tr>
</tbody>
</table>

Figure 6.32 The 5\textsuperscript{th} cycle stress-strain curve in tension direction for the cyclic tests with the strain amplitude of 0.6% at room temperature
The critical damage $D_{cr}$ is assumed to be temperature dependent and can be determined from the test data as follows:

First, determine the damage value in terms of elastic modulus degradation for the cyclic tests.

Second, calculate the dissipated energy for the cyclic testing according to the stress-strain hysteresis loop, then determine the damage value based on the internal entropy production (equation (3.81)).

Finally, determine $D_{cr}$ by matching the damage determined in terms of elastic modulus degradation with the internal entropy production-based damage.

In this thesis, $D_{cr}$ was determined from the cyclic tests with strain amplitude of 0.6% at various temperatures and was given as follows:

$$D_{cr} = -0.00545T + 0.659 \quad T \leq 100^\circ C$$  \hspace{1cm} (6.16)
6.4.2 Finite Element Simulation Results

For the cyclic tests with a strain amplitude of 0.6% at room temperature, the comparisons of the simulations for the uniaxial stress-strain hysteresis loop with experimental data at cycle 5, 50 and 104 are shown in figure 6.34, figure 6.35 and figure 6.36, respectively. For the cyclic tests with a strain amplitude of 0.6% at 75 °C, the comparisons of the simulations for the uniaxial stress-strain hysteresis loop with experimental data at cycle 5, 100 and 495 are shown in figure 6.37, figure 6.38 and figure 6.39, respectively. According to the simulation results, the proposed damage coupled viscoplasticity model performs very well except in compression. This is due to the fact that the values of parameters used in the simulations are determined in tension. However, the acrylic particulate composite exhibits markedly different inelastic behavior in tension and compression. The microstructure of the particulate composite consists of a distribution of ATH particles in a PMMA matrix. In tension, the ATH agglomerates act as stress concentrators, while in compression, the ATH agglomerates serve to transmit stresses. The resulting material is brittle in tension, but in compression it is similar in behavior to PMMA.
Figure 6.34 Uniaxial stress-strain hysteresis loop from simulation vs. experimental data for cycle 5 at room temperature with strain amplitude of 0.6%.

Figure 6.35 Uniaxial stress-strain hysteresis loop from simulation vs. experimental data for cycle 50 at room temperature with strain amplitude of 0.6%.
Figure 6.36 Uniaxial stress-strain hysteresis loop from simulation vs. experimental data for cycle 104 at room temperature with strain amplitude of 0.6%.

Figure 6.37 Uniaxial stress-strain hysteresis loop from simulation vs. experimental data for cycle 5 at 75 °C with strain amplitude of 0.6%.
Figure 6.38 Uniaxial stress-strain hysteresis loop from simulation vs. experimental data for cycle 100 at 75 °C with strain amplitude of 0.6%.

Figure 6.39 Uniaxial stress-strain hysteresis loop from simulation vs. experimental data for cycle 495 at 75 °C with strain amplitude of 0.6%.
The comparisons of the damage parameter obtained from the damage coupled viscoplastic model with that measured in tests in terms of elastic modulus degradation for the cyclic testing at room temperature and 75 °C are given in figure 6.40 and figure 6.41, respectively. The elastic modulus used for the calculation of the damage was determined according to figure 5.46. The simulation results are in good agreement with the experimental data. It is seen that most damage happens in the first few cycles, which is usually the reorganization of the initial manufacturing defects that can be introduced as the initial damage in the proposed model. Initial damage is probably due to the fact that particulate composites have many weak sites such as initial partial debonding between PMMA and ATH, agglomerates of ATH, which dominate the damage experienced in the first few cycles.

![Figure 6.40](image)

Figure 6.40 Comparison of damage parameter obtained from the damage coupled viscoplastic model with that measured in experiments in terms of elastic modulus degradation at room temperature with strain amplitude of 0.6%
The damage evolution law presented in this dissertation considers the damage as an isotropic internal state variable. This isotropic damage assumption is realistic in many cases especially under conditions of proportional loading when the principal stress directions remain unchanged (Lemaitre, 1996). The comparison of the damage parameter measured in terms of elastic modulus degradation with simulation results from the damage evolution function validates that the internal entropy production can be used as a criterion for damage. The improvement of the proposed model over the Basaran and Yan’s (1998) model is that a critical damage coefficient $D_{cr}$ is introduced to correlate disorder evolution with the material properties degradation.
6.4.3 Parametric Studies

The parametric study is based on the cyclic testing with a strain amplitude of 0.6% at room temperature. The influence of the parameters related to particulate composites on the damage evolution was studied.

The influence of CTE mismatch between the particle and the matrix on the damage of composite A at room temperature is shown in figure 6.42. Here, $T_c$ is the temperature that the residual stresses are set up in the microstructure due to the CTE difference between PMMA and ATH as cooling the composite from its curing temperature. These simulation results are obtained based on the assumption that the thickness of the interphase is 1% of the diameter of the particle and the elastic modulus of the interphase is 50% of that of PMMA. As seen in figure 6.42, CTE mismatch has negligible influence on the damage accumulation.

Figure 6.42 Effect of the CTE mismatch between the matrix and the particle on the damage of composite A at room temperature
The influence of stiffness of the interphase around the particle on the damage of composite A at room temperature is shown in figure 6.43. These results are obtained by only changing the young modulus of the interphase as the percentage of that of the matrix and keeping other parameters fixed ($T_c = 100^\circ C$ and the thickness of interphase is 1% of the diameter of particle). It is obtained that increasing the elastic modulus of the interphase increases the rate of damage.

![Figure 6.43 Effect of the stiffness of interphase around particle on the damage of composite A at room temperature](image)

The influence of thickness of the interphase around the particle on the damage of composite A at room temperature is shown in figure 6.44. These results are obtained by only changing the thickness of the interphase as percentage of the diameter of the particle.
and keeping other parameters fixed (\( T_c = 100^\circ C \) and the elastic modulus of the interphase is about 50% of that of PMMA). It is obtained that increasing the thickness of the interphase reduces the rate of damage.

![Graph showing the effect of the thickness of interphase on damage](image)

**Figure 6.44** Effect of the thickness of interphase around particle on the damage of composite A at room temperature

The influence of yield stress of composite A on the damage of composite A at room temperature is shown in figure 6.45. These results are obtained by only changing the isotropic hardening function of composite A and keeping other parameters fixed (\( T_c = 100^\circ C \) and the elastic modulus of interphase is about 50% of that of PMMA, thickness of interphase is 1% of diameter of filler). Increasing the yield stress decreases the damage rate and leads to longer fatigue life.
Figure 6.45 Effect of the yield strength of composite A on the damage of composite A at room temperature

The influence of the particle volume fraction on the damage of composite A at room temperature is shown in figure 6.46. These results are obtained by only changing the particle volume fraction and keeping other parameters fixed ($T_c = 100^\circ C$ and the elastic modulus of interphase is about 50% of that of PMMA, thickness of interphase is 1% of diameter of filler). Increasing the volume fraction of the particles increases the damage rate significantly.
Figure 6.46 Effect of the particle volume fraction on the damage of composite A at room temperature (Volume of Fraction (VoF))

The influence of the elastic modulus of the matrix on the damage of composite A at room temperature is shown in figure 6.47. These results are obtained by only changing the elastic modulus of the matrix and keeping other parameters fixed (T_e = 100°C and the elastic modulus of interphase is about 50% of that of PMMA, thickness of interphase is 1% of diameter of filler). Decreasing the elastic modulus of the composite decreases the damage rate.
The influence of the elastic modulus of the particle on the damage of composite A at room temperature is shown in figure 6.48. These results are obtained by changing only the elastic modulus of the particle and keeping other parameters fixed ($T_c = 100^\circ C$ and the elastic modulus of the interphase is about 50% of that of PMMA, the thickness of the interphase is 1% of diameter of filler). Decreasing the elastic modulus of the particles decreases the damage rate.
Figure 6.48 Effect of the elastic modulus of particle on the damage of composite A at room temperature

6.5 Thermal Cycling of a Composite Plate with a Cutout

The numerical simulations are performed for the thermomechanical fatigue behavior of a composite A plate with a cutout. The thermal loading profile and boundary conditions in the testing were used for the simulations. Only half of the plate is plotted and meshed for simulation due to the structural symmetry. A symmetric boundary condition is imposed on the left end of the half structure, and the bottom is supported in the vertical direction. The 4 sides of the plate are constrained by springs to prevent the plate from moving in the horizontal direction. The 8-node 3D thermomechanical element was used for the simulations. The half plate is shown in figure 6.49.
6.5.1 Model Parameters

The acrylic particulate composite is highly temperature and strain rate dependent especially near the glass transition temperature of the polymer. It is very important to determine the material parameters using the testing similar to the working environments of the products being simulated. In the current case, the plate was first uniformly heated up to 90 °C (at the control points) in 10 minutes and thus the temperature was kept at 90 °C for another 10 minutes, then the plate was cooled down by the fan located under the center of plate for 100 minutes. During the experiments, the strain at the corner (which is critical region for the plate), reached to 0.6% in 10 minutes, which is very slow. Therefore, the uniaxial tensile tests with lower strain rate are appropriate for determining the parameters needed in this simulations. Essentially, simulation and testing must be for
the same strain rate. Here, the uniaxial tensile testing data with a strain rate of $1 \times 10^{-5}$ per second are used to determine the parameters needed in the simulations. The damage coupled linear kinematic hardening model with linear isotropic hardening is used. The parameters for linear isotropic hardening and the linear kinematic model are determined as shown in figure 6.50 and figure 6.51, respectively. The initial yield stress and kinematic hardening modulus as a function of temperature was given in equation (6.17) and equation (6.18).

The critical damage parameter $D_{cr}$, which is depend on the temperature, loading profiles and magnitude, cannot be determined because of the lack of data for the plate with cutout. Here the value of 1 for $D_{cr}$ is used for the simulations and all the comparisons are based on $D_{cr} = 1$ compared to $D_{cr} = -0.00545T + 0.659$ used earlier for cycling loading.

![Initial Yield Stress vs Temperature](image)

Figure 6.50 Initial yield stress of composite A as a function of temperature
6.5.2 Finite Elements Simulation Results

According to the testing results of the plate with cutout, the critical regions with maximum strain and also maximum stress are at the corners of the cutout, which are close to the heating tub and therefore have a greater temperature gradient. Furthermore, the cracks always occur there during the cooling cyclic stage, when the tension field around the corners is produced. The simulation results for the strain in X direction as shown in figure 5.96 at the corners, which is believed to cause the cracks, are compared with the experimental measurements for the cycle 1, cycle 5, cycle 10 and cycle 34 as shown in figure 6.52, figure 6.53, figure 6.54 and figure 6.55, respectively.
Figure 6.52 Comparison of simulations with experimental measurements for strain in the plane direction at the corners close to heat source for cycle 1.

Figure 6.53 Comparison of simulations with experimental measurements for strain in the plane direction at the corners close to heat source for cycle 5.
Figure 6.54 Comparison of simulations with experimental measurements for strain in the plane direction at the corners close to heat source for cycle 10.

Figure 6.55 Comparison of simulations with experimental measurements for strain in the plane direction at the corners close to heat source for cycle 34.
The simulation results qualitatively agree with the experimental results but not quantitatively. The main reason for the difference between simulation and experimental results is due to the insensitivity of the model to tension and compression. The proposed model is isotropic and the parameters used in the model are determined from the uniaxial tensile tests. Acrylic particulate composites have very different thermomechanical properties between tension and compression. From our tests, creep in compression can be ignored in comparison of creep in tension. Also the yield strength in compression is 2-5 times of that in tension. The inelastic deformation in compression is negligible compared with that in tension at the same stress level. Therefore the damage caused by the entropy production in compression is negligible in comparison with the damage in tension. Moreover, the difference is part due to the approximate value of \( D_0 \) used in the finite element analysis.

An internal state variable, known as damage variable \( D \), is used to describe inherent microstructure degradation. The interaction between material degradation and mechanical response is considered by the damage coupled constitutive model developed in chapter 3 and chapter 4. Through numerical simulation, the evolution and distribution of damage can be obtained, which give a map of material degradation and a time history of damage evolution. The damage distribution provides important information for design optimization and product reliability. The damage distributions in the plate during the cooling stage for cycle 1, cycle 10 and cycle 34 are shown in figure 6.56, figure 6.57 and figure 6.58, respectively.
Figure 6.56 Damage distributions in the plate with cutout for cycle 1

Figure 6.57 Damage distributions in the plate with cutout for cycle 10
The von Mises stress is the standard measure of the stress intensity in the materials. The von Mises stress distributions in the plate during the cooling stage for cycle 1, cycle 10 and cycle 34 are also shown in figure 6.59, figure 6.60 and figure 6.61, respectively.
Figure 6.59 von Mises stress distributions in the plate with cutout for cycle 1

Figure 6.60 von Mises stress distributions in the plate with cutout for cycle 10
The simulation of damage parameter and von Mises stress at the corners of cutout as function of the number of cycles are also shown in figure 5.62 and figure 5.63, respectively.
Figure 6.62 Damage evolution at the corners close to the heat source as a function of the number of cycles.

Figure 6.63 von Mises stress at the corners close to the heat source as a function of the number of cycles.
6.5.3 Redesign of a Composite Plate with a Cutout

In the plate with cutout under thermal loadings, the corners of the cutout are the most critical regions, which determine the fatigue life of the plate. If we could reinforce the corners of the cutout using materials with high strength and stiffness such as steel, the fatigue life of the plate under thermal loadings will be improved greatly. For simplicity, here we use the steel as the reinforcing material, and the thermomechanical properties of steel are list as follows:

Elastic modulus: \( E_s = 200 \text{GPa} \)

Poisson’s Ratio: \( \nu_s = 0.29 \)

Specific heat: \( 1300 \text{J/kg} \cdot \text{K} \)

Thermal Conductivity \( 50 \text{W/m} \cdot \text{K} \)

Coefficient of thermal coefficient: \( \alpha_s = 1.5 \times 10^{-5} / \text{°C} \)

There may be many different ways to reinforce the corners of the cutout with steel. Here we consider the following two methods for reinforcing the corners of the cutout. The first method is shown in figure 6.64, where the reinforcing steel plate is placed in the inside of the corner and glued together with the surface of the corner. This method has a relatively high requirement for the production. However, the method will have good reinforcing effects because the steel directly reinforces the critical parts. Another method is shown in figure 6.65, where the reinforcing steel plate is placed on the top and bottom of the corner and glued together with the surfaces of the plate. This reinforcement is easy to make.
For comparison, the von Mises stress distributions from finite element analysis in the plate for the first cycle are shown in figure 6.66, figure 6.67 and figure 6.68 for the original plate without reinforcement (design #1), the plate with the reinforcing steel plate.
on the inside surface of the corner (design #2) and the plate with the reinforcing steel plate on the top and bottom surface at the corner (design #3), respectively. The comparison of the von Mises stress in the corner among all the three designs for the first cycle is shown in figure 6.69. It is obvious that the reinforcement can significantly decrease the stress in the corners, especially for design #2.

Figure 6.66 von Mises stress distributions around the corner close to the heat source for design #1
Figure 6.67 von Mises stress distributions around the corner close to the heat source for design #2

Figure 6.68 von Mises stress distributions around the corner close to the heat source for design #3
The material damage accumulates under fatigue loading, which is described by the damage variable in the proposed damage coupled viscoplastic model. When the overall damage in a material element reaches a critical value, the element is considered to be fully damaged resulting in the final rupture. Thus, the fatigue lifetime of the plate can be determined. The damage parameter evolution in the corners of the cutout as a function of the number of cycles is shown in figure 6.70 for all the designs. In addition, the von Mises stress in the corners of the cutout as a function of the number of cycles is shown in figure 6.71. Based on the value of the damage variable as shown in figure 6.70, the number of fatigue cycles for the reinforced plate with the cutout will be greatly improved compared to the plate without reinforcement.
Figure 6.70 Damage evolution in the corner close to the heat source as a function of the number of cycles

Figure 6.71 von Mises stress in the corner close to the heat source as a function of the number of cycles
7.1 Conclusions

Because of the low cost, ease of fabrication and improved material properties, acrylic particulate composites are being increasingly employed in a wide variety of domestic and industrial applications, thus creating a need to characterize their properties as well as understand their behavior under a variety of circumstances. The main aim of this dissertation was to characterize the failure mechanism and low cycle fatigue behavior of acrylic particulate composites, and investigate how the composite behavior is influenced by changes in certain parameters such as the interfacial bonding strength, the stiffness and thickness of the interphase, CTE mismatch between the matrix and the particle, and the volume fraction of the particles.

Due to the addition of rigid particles, interfacial debonding and filler agglomerate breakage are the dominant mechanism for the irreversible deformation, instead of crazing and shear yielding that are commonly associated with pure or homogeneous polymer systems. The influence of the interfacial bonding strength between the particle and the matrix on the failure mechanism of acrylic particulate composite has been investigated using in situ observations under uniaxial loading conditions. For acrylic particulate composites with weak interfacial bonding, the debonding, namely the separation of particles from the matrix, is the major damage mode. For acrylic particulate composites with strong interfacial bonding, the filler agglomerate breakage is the major damage
mode. Final fracture is produced by the incapacity of the matrix to carry loads released by the agglomerate of particles. It was shown that an increase in adhesive strength between the matrix and filler leads to an increase in strength at break. In contrast, weakening the interface between the matrix and filler results in a reduction in strength at break. An increase in adhesive strength between the matrix and the filler below certain critical bonding strength leads to a major reduction in the ductility. Surprisingly, continuous increase in adhesive strength above the critical bonding strength will improve the ductility of the particulate composite.

Experimental studies also demonstrated the significant influence of the interfacial bonding strength on the fatigue life of acrylic particulate composites. Under the strain controlled tests at the same conditions, composite A with the strongest interfacial bonding strength has a moderate fatigue life; composite B with the moderate interfacial bonding strength has the shortest fatigue life; composite C with the weakest interfacial bonding strength has the longest fatigue life. The elastic modulus degradation of an acrylic particulate composite under mechanical loading was measured. The damage was also characterized in terms of load-drop parameter, plastic strain range and hysteresis dissipation.

Flexural testing should not be used as a substitute for the measurement of the ultimate tensile strength in particulate composites; because the determination of stress is too complicated after the microporous zones (or cracks) are formed in particulate composites. Once the cracks occur, the uniformity of the beam is destroyed and the stresses in the beam are no longer related solely to the applied load and the specimen dimension. The relation between the peak load and the failure stress is obscure.
The mechanical properties of PMMA/ATH composite are strong functions of the temperature and strain rate. At room temperature, PMMA/ATH composite can be regarded as a rate insensitive material. At high temperature (close to glass transition temperature of PMMA), the viscoplastic properties must be considered. An important effect of the strain rate on the stress-strain curves of PMMA/ATH composite was also observed. Both the Young's modulus and the tensile strength increase as the strain rate increases.

Acrylic particulate composites have very different mechanical properties between tension and compression, including the ultimate strength, hardening modulus and creep behavior, which may be due to the different acting mechanism of reinforcing particles in tension and compression. The microstructure of the particulate composite consists of a distribution of ATH agglomerates in a PMMA matrix. In tension, the ATH agglomerates act as stress concentrators, while in compression the ATH agglomerates serve to transmit stresses.

Thermal cycling of a composite plate with a cutout was also performed. The accumulated strains on the corners of the cutout are measured using strain gages.

The internal state variable of damage corresponds to material degradation under fatigue loading. The internal entropy production, which is a measure of the irreversibility of the thermodynamic system, is used as the metric of damage. The damage evolution function was derived by making use of the basic concepts from two different disciplines, namely continuum mechanics and thermodynamics. The close correlation between the damage measured in terms of elastic modulus degradation and the damage obtained from the finite element simulation results validates the entropy based damage evolution
A micromechanical model for the effective elastic properties of particle filled acrylic composites with imperfect interfacial bonds is proposed. Particle filled acrylic composites are treated as three-phase composites consisting of the agglomerate of particles, the bulk matrix and the interfacial transition zone around the agglomerate. This is a very general model, which has coupled the following parameters: the volume fraction of particle, the properties of matrix and particle, the interfacial transition zone between the matrix and the filler, and the CTE mismatch between the matrix and the filler. The comparison of analytical simulation at macromechanical level with experimental data demonstrated the validity of the proposed micromechanical model with an imperfect interface.

A damage coupled viscoplastic constitutive model was also developed to characterize thermomechanical behavioral aspects of acrylic particulate composites. The damage coupled constitutive model reflects the interaction between damage and the mechanical response of composite material under thermomechanical loading. The material parameters involved in the constitutive model have been experimentally determined and have been implemented into the commercial finite element package ABAQUS through the user-defined subroutines. The finite element simulation results agree well with the test data of monotonic uniaxial tensile tests and low-cycle fatigue tests at various temperatures. It is shown that the proposed damage coupled viscoplastic
constitutive model can be used to predict the fatigue life of an acrylic particulate composite under thermomechanical fatigue loading.

7.2 Recommendations

Suggestions for future research related to the current work are summarized. Recommendations are made for the development of acrylic particulate composites with improved thermal stress resistance, as well as the directions to be taken in engineering design in order to reduce the susceptibility of acrylic particulate composite structures to thermal stress failure.

The model developed in this dissertation is an isotropic von Mises based model. However, the acrylic particulate composites usually have different properties in tension and compression. So it is advisable to develop an anisotropic model, which can account for the different behaviors, both in tension and compression.

The damage caused by thermomechanical loading in compression is negligible in comparison with the damage in tension. So the damage is not isotropic either. It is also advisable to expand the entropy based damage from scalar to tensor.

The CTE mismatch between the matrix and the particle is believed to have significant influence on the viscoplastic behavior of composites and is also coupled into the model. Surprisingly, the simulation results are not sensitive to the residual stress caused by the CTE mismatch between the matrix and the filler when cooling the composite from its peak polymerization temperature. This is due to the viscoplasticity constitutive model, which is based on the von Mises yield surface.
Creep has significant effects on the mechanical behavior of acrylic particulate composites. The creep flow function plays an important role in accounting for the rate-dependent behavior in the model. A series of creep tests are needed to characterize the rate-dependent properties of acrylic particulate composites. The model assumes the same creep properties both for the tension and compression, which is not the actual behavior. The simulation results should be improved if different creep properties in tension and compression are used.

High thermal conductivity is desirable in order to reduce heat build-up in the case of thermal shock. The addition of certain types of filler would enable such a compromise to be achieved. Many of the fillers which induce electrical conductivity also improve the thermal conductivity of plastic composites.

When considering the behavior of specimens with different interfacial properties in the case of the ATH-filled PMMA, it could be argued that for composite A with an adhesion promoting agent, the interfacial transition zone between the matrix and the filler is not the weak site. The agglomerate of particles is the weak site in the composite. So it may be more advantageous to improve the intergranular strength of the agglomerated particles rather than to improve the interfacial bonding strength between the filler and the matrix.

Both the experimental results and analytical predictions show that interfacial conditions have a significant influence on the elastic properties of particle filled acrylic composites. Based on these findings, it is reasonable to conclude that by controlling the interphase region thickness and elastic properties, it is possible to control the ductility and fatigue life of this particle filled composite. It is observed that increasing the interfacial
thickness would reduce the effective elastic modulus significantly, which would most likely lead to more ductile behavior and the fatigue life could be improved.

The simulation results for a plate with a cutout indicate that reinforcing the critical regions with material of high stiffness and strength, such as steel, can significantly improve the fatigue life of the composite plate made from particulate composite A. Furthermore, the closer the CTE of the reinforcing material is to that of particulate composite, the greater will be the reinforcing effects under thermal loads.

7.3 Contributions

- Improve the damage evolution model proposed by Basaran and Yan (1998);
- Expand Ju’ model (1996, 1997, 2001) to incorporate the damage parameter, imperfect interface bonding between the matrix and the filler, CTE mismatch between the matrix and the filler;
- Develop a micromechanical model for acrylic particulate composites consisting of the matrix, the filler and the transitional zone between the matrix and filler.
APPENDIX

Inverse of Fourth-Rank Tensor F

The product between two fourth-rank tensor $F(A_m)$ and $F(B_m)$, index $m = 1$ to 6, can be shown to follow:

$$F_{ijpq}(A_m)F_{pqkl}(B_m) = F_{ijkl}(C_m) \quad (A.1)$$

where $F$ is defined in equation (4.17) and

$$C_1 = A_1(B_1 + 4B_2 + B_3 + 2B_6) + 4A_2(B_1 + 2B_2 + B_3) + A_4(B_1 + 4B_2 + 3B_3) + 2A_5B_1 \quad (A.2)$$

$$C_2 = 2A_2(B_2 + B_3) + 2A_3B_2 \quad (A.3)$$

$$C_3 = A_3(B_1 + 4B_2 + B_3 + 2B_6) + A_5(B_1 + 4B_2 + 3B_3) + 2A_6B_3 \quad (A.4)$$

$$C_4 = A_1(B_4 + B_5) + 4A_2(B_4 + B_5) + A_4(B_4 + 3B_5 + 2B_6) + 2A_5B_4 \quad (A.5)$$

$$C_5 = A_3(B_4 + B_5) + A_5(B_1 + 3B_5 + 2B_6) + 2A_6B_5 \quad (A.6)$$

$$C_6 = 2A_5B_6 \quad (A.7)$$

To find the inverse of $F$, we recall the definition of the fourth-rank unit tensor $\delta_{ijkl}$

$$I_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \quad (A.8)$$

denoting by $F(A_m)$ the reverse tensor of $F(B_m)$, we can derive the components of $F(A_m) \equiv F^{-1}(B_m)$ by solving the system of equations (A.2) – (A.7) with the following arguments in $F(C_m)$

$$C_1 = C_2 = C_3 = C_4 = C_5 = 0 \quad C_6 = \frac{1}{2} \quad (A.9)$$
The results are

\[ A_6 = \frac{1}{4B_6} \]  \hspace{1cm} (A.10)

\[ A_2 = \frac{B_2}{4B_6(B_2 + B_6)} \]  \hspace{1cm} (A.11)

and

\[
\begin{bmatrix}
A_1 \\
A_4
\end{bmatrix} = D^{-1} \begin{bmatrix}
-2A_6B_4 - 4A_2(B_1 + 2B_2 + B_3) \\
-2A_6B_4 - 4A_2(B_4 + B_5)
\end{bmatrix}
\]

\[
\begin{bmatrix}
A_3 \\
A_5
\end{bmatrix} = D^{-1} \begin{bmatrix}
-2A_6B_3 \\
-2A_6B_5
\end{bmatrix}
\]

\[
\begin{bmatrix}
B_1 + 4B_2 + B_3 + 2B_6 & B_1 + 4B_2 + 3B_3 \\
B_4 + B_5 & B_4 + 3B_5 + 2B_6
\end{bmatrix}
\]

\hspace{1cm} (A.12)  \hspace{1cm} (A.13)  \hspace{1cm} (A.14)
REFERENCES


