Electromigration induced stress analysis using fully coupled mechanical–diffusion equations with nonlinear material properties

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Abstract

Electromigration is a major road block in the pursuit of further miniaturized electronics. In the next generation micro and sub micro electronics current density is expected to exceed $10^7$ A/cm². In this paper an electromigration induced strain-current density model is proposed and implemented in finite element procedure for solution of boundary/initial value electromigration problems. Numerical simulations are compared with experimental data. Comparisons validate the model.

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1. Introduction

Electromigration is a mass diffusion process as a result of an exchange of momentum between charge carriers and the thermally activated ions of the conductor [1]. Electromigration became of engineering interest since it was first observed as one of the primary failure mechanisms in aluminum IC conductors. Due to insatiable demand for miniaturization of electronics, electromigration induced failure is becoming a concern not only for IC thin films, but also for solder joints in micro-electronic systems [2–14]. Under high current density electromigration, vacancy diffusion is driven by four forces;

(1) electrical current field forces, which is due to momentum exchange between moving electrons and host atoms,
(2) stress gradient, due to accumulation and depletion of mass,
(3) temperature gradient, due to Joule heating,
(4) vacancy concentration gradient.

Most of the published works ignored the influence of third forces. Ye et al. [7] was the first to observe that temperature gradient driving force can be as strong as other forces and under some instances, a dominant force.

Blech and Sello [15] were the first to show that stress gradient can act as a counter force against electrical field driving force. As the mass moves from cathode side to anode side, compression on anode side and tension on cathode side will create a stress gradient. Black [16] was the first to establish a relationship between mean time to failure (MTTF) with current density, although he omitted many factors, hence it is applicable to certain specific cases he tested.

Numerous experiments have already proved the existence of a strain gradient within the thin film conductor line using X-ray diffraction which can penetrate the passivation layer on top of thin film [17–20]. Mechanical stress induced plastic deformation has been verified by the obvious evidence of whisker or hillock at the anode side of metal conductors [4–7,10,12,21]. Plastic deformation also contributes to the main damage phenomenon, which is void nucleation at the cathode side. Plastic deformation by grain boundary sliding produces high stress localization when the slip band intersects with particles at grain boundary, which is in favor of void nucleation. Also when there is stress, void growth may occur within grains as it is governed by power law creep [22]. Under high current density the damage is caused by several mechanisms including mechanical, thermal and electrical.

Physics literature is rich with empirical mean time to failure equations for thin films subject to electromigration. Yet these empirical and analytical equations can not be used for arbitrary boundary/initial value problems. Instead constitutive models that can be implemented in finite element method are needed [9,23,24]. Models proposed in the literature do not consider plastic deformation during electromigration process which cannot be neglected. Also real interaction of vacancy flux and stress, which exists concurrently, needs to be solved together and not by a sequential method as it is conventionally done in the literature [24], because of the coupled effect between stress evolution and atomic flux. In this paper, a fully coupled model for simulation of mechanical stress and vacancy diffusion with inelastic mechanical material property is proposed. The model accounts for vacancy flux due to electromigration, stress gradient, thermomigration and vacancy concentration gradient. In depth literature survey of existing electromigration models can be found in Basaran et al. [25].

2. Physical model

There are several electromigration stress evolution models proposed in the literature. Kirchheim [26] proposed a stress model for electromigration in which generation of tensile and compressive stresses in grain boundaries during electromigration is caused by the transport, annihilation and generation of vacancies. Self-consistent equations were proposed describing vacancy migration through a grain boundary and the associated stress evolution. Another physical model was proposed by Korhonen et al. [27] to describe the mechanical stresses arising due to electromigration in a confined thin film deposited on an oxidized silicon substrate and covered by a rigid dielectric passivation layer. Korhonen's model's biggest disadvantages are that vacancy relaxation effect was not taken into account and vacancy equilibrium was assumed. Based on Kirchheim and Korhonen's work, Sarychev and Zhinikov [28] proposed another stress model which connects the evolution of the stress tensor with the transport of vacancies, the geometry of the metallization and the stress and displacement boundary conditions that apply to it.

And he gave out several analytical solutions based on elastic material properties and special boundary conditions. It should be pointed out that none of the three models mentioned above include thermomigration, which cannot be neglected under some circumstances as pointed out by Ye
et al. [7]. Also these models all assume that material is elastic. We base our constitutive modeling on Sarychev’s stress evolution model. Because of Sarychev’s model is based on vacancy concentration not atomic concentration, the flux in the later formulation is refer to vacancy flux instead of atomic flux.

3. Finite element formulation

The proposed model is implemented with ABAQUS general purpose finite element program using thermal-displacement analysis option. ABAQUS and other commercially available finite element codes do not have the capability to solve general electromigration problem directly. Thermal-displacement option is used simply because from a mathematical point of view, diffusion process and thermal flux is governed by the same type of parabolic differential equations. With the ABAQUS user element interface, we can embed the program into ABAQUS, where the temperature degree of freedom is utilized for normalized concentration of vacancy. An 8-node quadratic 2D element and a twenty-node 3D brick element have been established to simulate both 2D and 3D electromigration boundary value problems.

In the following presentation of the model development, we adopt viscoplastic material behavior with kinematic and isotropic hardening which can accommodate most metal mechanical properties. The ultimate goal of this project is to study electromigration induced damage on microelectronics solder joints, which exhibit highly viscoplastic behavior with nonlinear kinematic/isotropic hardening. Ye et al. [10] have shown that solder joints under high current density exhibit significant viscoplastic behavior.

3.1. Governing equations

Electromigration is a diffusion controlled mass transport process. It is governed by the following vacancy conservation equation which is equivalent to mass conservation equation.

\[ \int_v \left( C_{v0} \frac{\partial c}{\partial t} + \nabla \cdot q - G \right) dV = 0 \]  

(1)

where

- \( C_{v0} \) is equilibrium vacancy concentration in the absence of stress field,
- \( c \) is normalized vacancy concentration and \( c = c_{v}/c_{v0} \),
- \( c_{v} \) is vacancy concentration,
- \( t \) is time,
- \( q \) is vacancy flux,
- \( G \) is vacancy generation/annihilation rate.

Force equilibrium is governed by the following equation

\[ \frac{\partial \sigma_{ij}}{\partial x_j} = 0 \]  

(2)

3.2. Constitutive equations

Assuming that driving forces of vacancy flux are vacancy concentration gradient, electrical field forces, stress gradient and thermal gradient, the vacancy flux is given by [25,26,28]

\[ q = -D_{v} C_{v0} \left( \nabla c + Z^* e \frac{kT}{\rho} (-\rho) c + \frac{c f }{kT} \nabla \sigma_{\text{spherical}} + \frac{c}{kT^2} Q^* \nabla T \right) \]  

(3)

where

- \( D_{v} \) is vacancy diffusivity,
- \( Z^* \) is vacancy effective charge number,
- \( e \) is electron charge,
- \( \rho \) is metal resistivity,
- \( j \) is current density (vector),
- \( f \) is vacancy relaxation ratio, ratio of atomic volume to the volume of a vacancy,
- \( \Omega \) is atomic volume,
- \( k \) is Boltzmann’s constant,
- \( T \) is absolute temperature,
- \( \sigma_{\text{spherical}} \) is spherical part of stress tensor,
- \( \sigma_{\text{spherical}} = \text{trace}(\sigma_{ij})/3 \).

\( Q^* \) is heat of transport, the isothermal heat transmitted by moving the atom in the process of jumping a lattice site less the intrinsic enthalpy.
The stress–vacancy relationship is represented by vacancy generation/annihilation rate which is given by [28]

\[ G = -C_v \frac{c - C_{ve}}{\tau_v} \tag{4} \]

Eq. (4) goes back to the work by Rosenberg and Ohring [29] and is also used by Kirchheim [26]. It is pointed out by Kirchheim that the equation is only valid for small deviation from the equilibrium concentration of vacancies, for larger deviation which occur in the depletion zone of a stressed line it should be replaced by another equation [30], where \( C_{ve} = e^{-\left(1 - \frac{kT}{s} \right)} \) is normalized thermodynamic equilibrium vacancy concentration.

\( \tau_v \) is characteristic vacancy generation/annihilation time.

Stress is governed by

\[ \sigma = K_{\text{Stiffness}} \varepsilon \tag{5} \]

where \( K_{\text{Stiffness}} \) is the tangential stiffness matrix.

### 3.3. Discretization for finite element method implementation

With Eq. (1) using weighted residues method, we can write the following relationship,

\[ \int_D \varepsilon \left[ C_{\varepsilon} \left( \varepsilon \frac{\partial c}{\partial t} + \nabla \cdot \mathbf{q} - G \right) \right] dV = 0 \tag{6} \]

Using integration by parts and divergence theorem, we obtain

\[ \int_D \varepsilon \cdot \nabla \cdot \mathbf{q} dV = - \int_D \varepsilon \frac{\partial \varepsilon}{\partial t} \cdot \mathbf{q} dV + \int_S \varepsilon \cdot \mathbf{q} \cdot \mathbf{n} dS \tag{7} \]

Substitute (7) into (6) and using normalized flux and vacancy generation rate to eliminate \( C_v \)

\[ \int_D \varepsilon \cdot \frac{\partial \varepsilon}{\partial t} dV = - \int_D \varepsilon \frac{\partial \varepsilon}{\partial t} \cdot \mathbf{q} dV \]

\[ = - \int_S \varepsilon \cdot \mathbf{q} \cdot \mathbf{n} dS + \int_D \varepsilon \mathbf{G} dV \tag{8} \]

If we assume blocking boundary condition for vacancy flux, \( \mathbf{q} \cdot \mathbf{n} = 0 \) then substituting constitutive equations (3) and (4) into (8), we obtain

\[ \int_D \varepsilon \frac{\partial \varepsilon}{\partial t} dV + \int_D \varepsilon \frac{\partial \varepsilon}{\partial t} \cdot \mathbf{D} \]

\[ \cdot \left( \nabla \varepsilon + \frac{Z^* e}{kT} (-\rho \mathbf{c}) + \frac{c f Q}{kT} \nabla \sigma_{\text{spherical}} + \frac{c}{kT} Q' \nabla T \right) dV \]

\[ - \int_D \varepsilon \cdot \frac{e^{-\left(1 - \frac{kT}{s} \right)}}{\tau_v} - \varepsilon dV = 0 \tag{9} \]

The Galerkin approach assumes that, the variational field, is interpolated by the same functions as weight functions used for method of weighted residuals.

\[ \delta \varepsilon = N^T \delta \varepsilon \tag{10} \]

\[ \left[ \int_D \varepsilon \frac{\partial \varepsilon}{\partial t} \cdot D \left( \nabla \varepsilon + \frac{Z^* e}{kT} (-\rho \mathbf{c}) + \frac{c f Q}{kT} \nabla \sigma_{\text{spherical}} + \frac{c}{kT} Q' \nabla T \right) dV \right] \delta \varepsilon = 0 \]

\[ \left[ \int_D \varepsilon \frac{\partial \varepsilon}{\partial t} \cdot D + \int_D N^T \frac{\partial \varepsilon}{\partial t} \cdot dV + \int_D N^T \varepsilon dV \right] \delta \varepsilon = 0 \tag{11} \]

Discretization of force equilibrium equation (2) can be found at any finite element text book so it is omitted here.

It should emphasize that for a general solution of Eq. (11) temperature gradient term in Eq. (11) should also be discretized in space. Yet doing so, yields an extra nodal unknown in addition to three displacements, one vacancy concentration d.o.f that results from other terms in this equation, which ABAQUS cannot solve when an element has five nodal unknowns. As a first order approximation, the temperature gradient field can be obtained from a separate thermal analysis. Because thermal steady state is usually established much faster than vacancy diffusion process, steady state temperature gradient from thermal analysis can be used for this term.

### 3.4. Integration algorithm

The complexity of this problem comes from coupling terms between diffusion governing equation and force equilibrium governing equation and coupling between temperature gradient and diffusion governing equation. As a first step the latter coupling is ignored. In order to determine Jacobian contributions material constitutive equation is needed. Because of the nonlinear behavior of the material (viscoplasticity), a local integration scheme is also needed, here return mapping
algorithm [31] is used. In the following derivation current step means at step \( n + 1 \), the state variables at previous step \( n \) are known.

The stress–strain constitutive model is established as

\[
\sigma = K_{\text{Stiffness}} (\varepsilon_{\text{total}} - \varepsilon_{\text{viscoplastic}} - \varepsilon_{\text{electromigration}} - \varepsilon_{\text{thermal}})
\]

where \( K_{\text{Stiffness}} = \kappa \mathbf{1} \otimes \mathbf{1} + 2\mu (\mathbf{I} - \frac{1}{3} \mathbf{1} \otimes \mathbf{1}) \) and \( \kappa \) is bulk modulus, \( \mu \) is shear modulus; and

\[
\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{I} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}
\]

\( \varepsilon_{\text{electromigration}} = \frac{1}{3} \mathbf{1} \cdot \varepsilon_{\text{trace}} \)

Thermal strain is not included as a field variable in current formulation but it can be added into the model from the results of an independent thermal-displacement analysis.

Itemized strain components,

\[
\varepsilon_{\text{total}} = \frac{1}{3} \varepsilon_{\text{trace}} \cdot \mathbf{1} + \varepsilon_{\text{dev}}
\]

\[
\varepsilon_{\text{viscoplastic}} = \frac{1}{3} \varepsilon_{\text{trace}} \cdot \mathbf{1} + \varepsilon_{\text{dev}}
\]

\[
\varepsilon_{\text{electromigration}} = \frac{1}{3} \varepsilon_{\text{trace}} \cdot \mathbf{1} + \varepsilon_{\text{dev}}
\]

Substitute Eqs. (13)–(15) into Eq. (12), we obtain

\[
\sigma = K \cdot (\varepsilon_{\text{trace}} - \varepsilon_{\text{electromigration}}) \cdot \mathbf{1} + 2\mu (\varepsilon_{\text{dev}} - \varepsilon_{\text{viscoplastic}})
\]

where \( \varepsilon_{\text{electromigration}} \) is described by following equation [28]

\[
\frac{\partial \varepsilon_{\text{electromigration}}}{\partial t} = \Omega C_{\varepsilon_{\text{electromigration}}}(f \nabla q + f'G)
\]

\[ f' = 1 - f \]

According to Eq. (17), it is assumed that when an atom is replaced by a vacancy there is a local spherical strain introduced at that lattice site due to difference between the volume of an atom and volume of a vacancy. Electromigration introduced strain happens due to

(1) vacancy flux divergence,

(2) vacancy generation.

Using Eq. (1), we can transform Eq. (17) into

\[
\frac{\partial \varepsilon_{\text{electromigration}}}{\partial t} = \Omega C_{\varepsilon_{\text{electromigration}}}(G - f \frac{\partial \varepsilon_{\text{electromigration}}}{\partial t})
\]

\[
= \Omega C_{\varepsilon_{\text{electromigration}}}(G) - c - \frac{\partial \varepsilon_{\text{electromigration}}}{\partial t}
\]

Eqs. (16) and (18) plus \( J_2 \) plasticity theory combined together yield the constitutive material behavior.

Now we perform a local integration scheme to determine the stiffness matrix \( \varepsilon_{\text{trial} n+1} \) and update the plastic strain and other related state variables.

First, we establish a trial state which we assumed elastic behavior at current step \( n + 1 \)

\[
\varepsilon_{\text{trial} n+1} = 2\mu \cdot \left( \mathbf{1} - \frac{1}{3} \mathbf{1} \otimes \mathbf{1} \right) (\varepsilon_{\text{dev} n+1} - \varepsilon_{\text{dev} n})
\]

where \( s \) is the deviatoric stress. And viscoplastic flow is described by flow rule as

\[
\dot{\varepsilon} = \gamma \mathbf{n}
\]

with \( \mathbf{n} = \frac{\partial \varepsilon_{\text{electromigration}}}{\partial t} \) which is normal to the yield surface, where \( \gamma \) is the consistency parameter.

Consider kinematic hardening, we define relative effective stress as

\[
\sigma_{\varepsilon_{\text{trial} n+1}} = \sigma_{\varepsilon_{\text{trial} n+1}} - X_n
\]

where \( X_n \) is back stress tensor and \( X_n \) is described as

\[
\frac{\partial X}{\partial t} = \gamma \frac{2}{3} H'(\xi) \frac{\xi}{||\xi||}
\]
\[ \dot{\varepsilon} = \sqrt{\frac{2}{3}} \gamma \]  
(23)

where \( H'(\gamma) \) is kinematic hardening modulus.

\( \gamma \) is equivalent plastic strain given by

\[ \gamma = \frac{\langle \phi(F) \rangle}{\eta} \quad \text{(28)} \]

\[ F = \Theta \left( \frac{\Delta \gamma \eta}{\Delta t} \right) \quad \text{(29)} \]

where

\[ \Theta \left( \frac{\Delta \gamma \eta}{\Delta t} \right) = \phi^{-1} \left( \frac{\Delta \gamma \eta}{\Delta t} \right) \]

and \( \Delta \gamma = \gamma_{n+1} - \gamma_n \), which is based on implicit backward difference scheme.

Tang and Basaran [32] developed viscoplastic flow rule for solder alloys based on Kashyap and Murty [33] model, where grain boundary sliding is the dominant mechanism, primary and steady state creep can be given by

\[ \dot{b}_{ij}^{yp} = \frac{AD_0 Eb}{k \theta} \left( \frac{\langle F \rangle}{E} \right)^n \left( \frac{b}{d} \right)^p \exp^{-Q/(k \theta)} \frac{\partial F}{\partial \sigma_{ij}} \]  
(30)

where the material parameters are defined as follows,

\( A \) a dimensionless material parameter to describe the strain rate sensitivity,

\( D_0 \) is a frequency factor,

\( Q \) is the creep activation energy for plastic flow,

\( R \) is the universal gas constant = 8.314 J/K mol = 8.314 N mm/K mol,

\( \theta \) absolute temperature in K,

\( E \) Young’s modulus,

\( b \) characteristic length of crystal dislocation (magnitude of Burger’s vector),

\( k \) Boltzmann’s constant,

\( d \) average phase size,

\( p \) grain size exponent,

\( n \) stress exponent for plastic deformation rate, where \( 1/n \) indicates strain rate sensitivity.

From (20), (28) and (30), we can identify,

\[ \langle \phi(F) \rangle = \langle F \rangle^n \]  
(31)

\[ \frac{1}{\eta} = \frac{AD_0 Eb}{k \theta} \left( \frac{1}{E} \right)^n \left( \frac{b}{d} \right)^p \exp^{-Q/(k \theta)} \]  
(32)

If \( f_{n+1}^{\text{trial}} \leq 0 \) then set \( s_{n+1}^{\text{trial}} = s_{n+1} \); Otherwise there is plastic strain at current step, using flow rule equation (20), \( S_{n+1} \) and \( \xi_{n+1} \) can be obtained as follows:

\[ S_{n+1} = S_{n+1}^{tr} - \Delta \gamma 2 \mu n_{n+1} \]  
(33)

\[ \| \xi_{n+1} \| + \left\{ \Delta \gamma 2 \mu + \sqrt{\frac{2}{3} A H} \right\} = \| \xi_{n+1}^{tr} \| \]  
(34)

where

\[ n_{n+1} = \frac{\xi_{n+1}^{tr}}{\| \xi_{n+1}^{tr} \|} \]  
(35)

Using (24) for the rate independent case or (29) for the rate dependent case we have the following nonlinear scalar equation for the consistency.
parameter which can be solved by a local Newton method [31], where $g(\Delta \gamma)$ is a scalar equation with the only unknown $\Delta \gamma$,

$$g(\Delta \gamma) = -\sqrt{\frac{2}{3}} K(x) + \| \xi_{n+1} \|
- \left[ \Delta \gamma 2\mu + \sqrt{\frac{2}{3}} \Delta H_{n+1} \right] - \Theta \left( \frac{\Delta \gamma H}{\Delta \gamma} \right) = 0$$

(36)

Once (36) is solved for $\Delta \gamma$ using the following updating scheme [31]

$$x_{n+1} = x_n + \sqrt{2/3} \Delta \gamma$$  
(37)

$$\xi_{n+1} = \xi_{n} + \Delta \gamma n_{n+1}$$  
(38)

$$X^D_{n+1} = X^D_n + \frac{2}{3} H'(x_{n+1}) \Delta \gamma n_{n+1}$$  
(39)

$$\xi_{n+1} = R(x_{n+1}) n_{n+1}$$  
(40)

$$S_{n+1} = \xi_{n+1} + X^D_{n+1}$$  
(41)

$$\sigma_{n+1} = S_{n+1} + \frac{1}{3} \text{Tr}(\sigma_{n+1}) I = S_{n+1} + \sigma_{n+1}^{\text{spherical}}$$  
(42)

$$\sigma_{n+1}^{\text{spherical}}$$ is determined as follow equation

$$\sigma_{n+1}^{\text{spherical}} = \sigma_{n}^{\text{spherical}} + \kappa (\text{Tr}(\Delta \sigma_{n+1}^{\text{total}}) - \text{Tr}(\Delta \sigma_{n+1}^{\text{electromigration}}))$$  
(43)

According to rate equation of (17),

$$\text{Tr}(\Delta \sigma_{n+1}^{\text{electromigration}}) = \Omega C_{i0} \left( \frac{(1-M)\sigma_{n+1}^{\text{spherical}}}{\tau_s} - C_{n+1} - f \Delta c \right)$$  
(44)

Substitute (44) into (43) and after some manipulation we can get

$$\sigma_{n+1}^{\text{spherical}} = \sigma_{n}^{\text{spherical}} - \kappa \left[ \text{Tr}(\Delta \sigma_{n+1}^{\text{total}}) - \Omega C_{i0} \left( \frac{(1-M)\sigma_{n+1}^{\text{spherical}}}{\tau_s} - C_{n+1} - f \Delta c \right) \right] = 0$$

(45)

Iterating above scalar equation we get updated spherical stress and substitute updated spherical stress into (42), we obtain updated stress at step $n + 1$.

3.5. Contributions of Jacobian

Now we can determine consistent stiffness matrix through linearization of Eq. (16), with differentiating both side of the equation:

$$k_{n+1} = \kappa \cdot \left( I - \frac{1}{2} \frac{\partial \sigma_{n+1}^{\text{trace}}}{\partial \sigma_{n+1}} \right) + 2\mu \frac{\partial (h_{\text{total},n+1} - h_{\text{VP},n+1})}{\partial \sigma_{n+1}}$$

(46)

with some basic manipulation and noting that

$$\frac{\partial h_{\text{total},n+1}}{\partial \sigma_{n+1}} = (I - \frac{1}{2} I \otimes I)$$

and

$$\frac{\partial h_{\text{VP},n+1}}{\partial \sigma_{n+1}} = \frac{\partial \sigma_{n+1}^{\text{VP}}}{\partial \sigma_{n+1}}$$

the second part of equation (1.46) can be described as [31]

$$k'_{n+1} = 2\mu \left( I - \frac{1}{3} I \otimes I \right) + 2\mu \cdot \frac{\partial \sigma_{n+1}^{\text{VP}}}{\partial \sigma_{n+1}}$$

(47)

With

$$\frac{\partial \sigma_{n+1}^{\text{VP}}}{\partial \sigma_{n+1}} = \kappa \left[ \frac{2}{\tau_s} + K(x_{n+1}) + H'(x_{n+1}) \right] \frac{\sigma_{n+1}^{\text{VP}}}{3\mu}$$

(48)

and

$$\frac{\partial \sigma_{n+1}^{\text{VP}}}{\partial \sigma_{n+1}} = \frac{n_{n+1}}{\| n_{n+1} \|} \left( I - \frac{1}{3} I \otimes I - n_{n+1} \otimes n_{n+1} \right)$$

(49)

The integration detail for Eq. (47) is given by Simo and Hughes [31].

Substitute (48) and (49) into (47),

$$k'_{n+1} = 2\mu (0_{n+1} \cdot (I - \frac{1}{3} I \otimes I) - \bar{\sigma}_{n+1} n_{n+1} \otimes n_{n+1})$$

(50)

with

$$\bar{\sigma}_{n+1} = 1 - \frac{\Delta \gamma 2\mu}{\| \xi_{n+1} \|}$$

(51)

and

$$\bar{\sigma}_{n+1} = \frac{\Omega C_{i0}}{2n} \bar{\sigma}_{n+1} + \frac{k'(x_{n+1}) + H'(x_{n+1})}{3\mu} - \frac{\Delta \gamma 2\mu}{\| \xi_{n+1} \|}$$

(52)
Now we return to Eq. (46) to determine consistent stiffness matrix at step $n + 1$, with Eqs. (43) and (44), we can get nine equations with nine unknowns as follow

$$
k_{ij}^{n+1} = \kappa \left( 1 - \Omega \Delta t \sum_{k=1}^{3} k_{ij}^{k} \right) + k_{ij}^{n+1}
$$

(53)

where $\Xi = \frac{C_0 \beta \Omega}{3 \kappa} \left( \frac{1 - f}{\Delta t} \right)$. (54)

Solve above symmetric equation to obtain final form of the stiffness matrix

$$
k_{ij}^{n+1} = \kappa \left[ 1 - \Omega \Delta t \Xi \left( 3 \kappa - \kappa \Omega \Delta t \Xi \frac{9 \kappa + k_{ij}^{\text{total}}}{1 + 3 \kappa \Omega \Delta t \Xi} + \sum_{k=1}^{3} k_{ij}^{k} \right) \right] + k_{ij}^{n+1}
$$

(54)

where $k_{ij}^{\text{total}} = \sum_{i,j=1}^{3} k_{ij}^{(i,j)}$ for $i,j = 1,3$ for other terms of $k_{ij}^{n+1}$ it is defined by

$$
k_{ij}^{n+1} = k_{ij}^{n+1}
$$

(55)

for $i,j = 4,6$.

Other terms of constitutive model needed for final total Jacobian matrix can be derived from $k_{ij}^{n+1}$.

We will derive those as follows.

Based on Eqs. (16) and (18) we can get

$$
\frac{\partial \sigma}{\partial \epsilon_{n+1}} = \kappa C_0 \Omega \delta_{ij} \left( \Delta t \frac{\partial G}{\partial \epsilon_{n+1}} - \frac{f \partial \Delta \epsilon_{n+1}}{\partial \epsilon_{n+1}} \right)
$$

(56)

Substitute $G$ and notice that $\frac{\partial \Delta \epsilon_{n+1}}{\partial \epsilon_{n+1}} = 1$, we can obtain three equations with three unknowns

$$
\frac{\partial \sigma_{n+1}}{\partial \epsilon_{n+1}} = -\delta_{ij} \kappa \Omega C_0 \left( \frac{\Delta t}{\tau_x} - f \right) + \delta_{ij} \kappa \Omega C_0 \Delta t
$$

$$
\times \frac{(1 - f) \Omega}{3 \kappa \tau_x} \left( \frac{1 - f}{\Delta t} \right) \sum_{i,j=1}^{3} \delta_{ij} \frac{\partial G_{ij}^{n+1}}{\partial \epsilon_{n+1}}
$$

(57)

We solve above equations to obtain

$$
\frac{\partial \sigma_{n+1}^{ij}}{\partial \epsilon_{n+1}^{ij}} = \kappa \Omega C_0 \left( \frac{\Delta t}{\tau_x} - f \right)
$$

$$
+ \frac{3 \kappa \Omega C_0 \Delta t}{3 \kappa \Omega C_0 \Delta t} e^{(1 - f) \Omega \sigma_{n+1}^{ij} \frac{1 - f}{\Delta t}}
$$

(58)

By using Eq. (3), we can get

$$
\frac{\partial \mathbf{q}_{n+1}}{\partial \epsilon_{n+1}^{ij}} = -D \left( \frac{\partial}{\partial \mathbf{x}} + \frac{Z^e}{kT} (\mathbf{p}) + \frac{f \Omega \nabla \frac{\partial \sigma_{n+1}^{spherical}}{\partial \epsilon_{n+1}^{ij}}}{kT} + \frac{Q \nabla \mathbf{q}_{n+1}}{kT^2} \right)
$$

(59)

Where all terms are known except for the term $\frac{\partial \sigma_{n+1}^{spherical}}{\partial \epsilon_{n+1}^{ij}}$, which can be calculated using finite difference scheme at local material points. Then it can be reformed as

$$
\frac{\partial \nabla \sigma_{n+1}^{spherical}}{\partial \epsilon_{n+1}^{ij}} = \frac{\partial}{\partial \mathbf{x}} \left( \frac{\partial \sigma_{n+1}^{spherical}}{\partial \epsilon_{n+1}^{ij}} \right)
$$

(60)

where $\frac{\partial \sigma_{n+1}^{spherical}}{\partial \epsilon_{n+1}^{ij}}$ can be calculated from (58).

Also we can derive the following relation from Eq. (3)

$$
\frac{\partial \mathbf{q}_{n+1}}{\partial \epsilon_{n+1}^{ij}} = -D \left( \frac{\partial}{\partial \mathbf{x}} + \frac{Z^e}{kT} (\mathbf{p}) + \frac{f \Omega \nabla \frac{\partial \sigma_{n+1}^{spherical}}{\partial \epsilon_{n+1}^{ij}}}{kT} + \frac{Q \nabla \mathbf{q}_{n+1}}{kT^2} \right)
$$

(61)

where $(\frac{\partial \sigma_{n+1}^{spherical}}{\partial \epsilon_{n+1}^{ij}})$ is given by (54).

From Eq. (4), we can obtain

$$
\frac{\partial G_{n+1}}{\partial \epsilon_{n+1}^{ij}} = \left( \frac{\partial \epsilon_{n+1}^{ij}}{\partial \epsilon_{n+1}^{ij}} \right) \frac{(1 - f) \Omega}{kT} \frac{\partial \sigma_{n+1}^{spherical}}{\partial \epsilon_{n+1}^{ij}} - \frac{1}{\tau_s}
$$

(62)

where $\frac{\partial \epsilon_{n+1}^{ij}}{\partial \epsilon_{n+1}^{ij}}$ is given out through Eq. (58)

Also from Eq. (4), we can obtain

$$
\frac{\partial G_{n+1}}{\partial \epsilon_{n+1}^{ij}} = \left( \frac{\partial \epsilon_{n+1}^{ij}}{\partial \epsilon_{n+1}^{ij}} \right) \frac{(1 - f) \Omega}{kT} \frac{\partial \sigma_{n+1}^{spherical}}{\partial \epsilon_{n+1}^{ij}} - \frac{1}{\tau_s}
$$

(63)

With Eqs. (54), (55), (58)–(63), we have got all the terms needed for calculating the final Jacobian terms at current step $n + 1$.

First taking derivative with respect to $c$ for Eq. (11), we obtain

$$
k_{cc}^{1} = \int \int \int \frac{1}{\Delta t} \cdot N \cdot dV
$$

(64)

$$
k_{cc}^{2} = \int \int \int \frac{\partial N \cdot N}{\partial \mathbf{x}} \cdot D \cdot \left( \frac{\partial \epsilon_{n+1}^{ij}}{\partial \epsilon_{n+1}^{ij}} \right) \frac{(1 - f) \Omega}{kT} \frac{\partial \sigma_{n+1}^{spherical}}{\partial \epsilon_{n+1}^{ij}} \cdot N + \frac{Q \nabla \mathbf{q}_{n+1}}{kT^2} \cdot N
$$

(65)
\[
\begin{align*}
    k_{cc}^3 &= \int \int \int \psi \left( \begin{array}{c}
    (1-f) \frac{\Omega}{kT} e^{-\frac{(1-f)(\sigma_{n+1}^{\text{spherical}})}{kT}} - 1 \\
    \tau_x
\end{array} \right) \cdot N dV \quad (66)
\end{align*}
\]

and we have
\[
    k_{cc}^{n+1} = k_{cc}^1 + k_{cc}^2 + k_{cc}^3 \quad (67)
\]

Also we can take derivative with \( u^M \) for Eq. (11), we can obtain
\[
\begin{align*}
    k_{cu}^{1} &= \int \int \int \psi \cdot \frac{\partial \sigma_{n+1}^{\text{spherical}}}{\partial \epsilon_x} \cdot \frac{1-f}{kT} \cdot \frac{\partial \Omega}{\partial \epsilon_x} \cdot \frac{\partial \sigma_{n+1}^{\text{spherical}}}{\partial \sigma_{n+1}^{\text{spherical}}} \\
    &\quad \cdot B dV \quad (68)
\end{align*}
\]

where \( \epsilon_{n+1}^M = B \otimes u^M \)
\[
\begin{align*}
    k_{cu}^{2} &= \int \int \int \psi \cdot \frac{\partial \sigma_{n+1}^{\text{spherical}}}{\partial \epsilon_x} \cdot \frac{1-f}{kT} \cdot \frac{\partial \Omega}{\partial \epsilon_x} \\
    &\quad \cdot \frac{\partial \sigma_{n+1}^{\text{spherical}}}{\partial \epsilon_{n+1}^{\text{spherical}}} \cdot B dV \quad (69)
\end{align*}
\]

and
\[
    k_{cu}^{n+1} = k_{cu}^1 + k_{cu}^2 \quad (70)
\]

At the same time, we can also take derivative with regard to the discretized displacement governing equation, we obtain:
\[
\begin{align*}
    k_{uu}^{n+1} &= \int \int \int \psi \cdot B^T \otimes k_{n+1} \otimes B dV \\
    &= \int \int \int \psi \cdot B^T \otimes B \otimes B dV \\
    &= \int \int \int \psi \cdot B dV \quad (71)
\end{align*}
\]

Finally, we have our final Jacobian matrix as
\[
    K_{n+1} = \left[ \begin{array}{cccc}
    k_{cc}^{n+1} & k_{cu}^{n+1} & k_{uc}^{n+1} \\
    k_{cu}^{n+1} & k_{uu}^{n+1} & k_{mu}^{n+1}
    \end{array} \right] \quad (73)
\]

4. Verification of the proposed model

4.1. Mesh sensitivity

There are many experiments reported in the literature calculating stress based on elastic strain measurement during electromigration. In order to eliminate thermal stress contribution, we choose Valek’s [21] experiment to verify our model because it reports the deviatoric stress which eliminates thermal stress influence. Valek uses scanning white beam X-ray microdiffraction, which allows for mapping the complete orientation and deviatoric strain tensor of micron-scale grains within a passivated thin film interconnect line.

The geometry of Valek’s experiment is an aluminum thin film of 4.1 \( \mu \text{m} \) of width, 30 \( \mu \text{m} \) in length and 0.75 \( \mu \text{m} \) in thickness. It is passivated by 0.7 \( \mu \text{m} \) of SiO\textsubscript{2} on both sides. Current was ramped up to 30 mA (\( j = 0.98 \text{ MA/cm}^2 \)) over the course of 24 h with increments of 10 mA, then turn off for 12 h. The material used for samples is sputtered Al (0.5 wt.% Cu). During the experiment the temperature is controlled at 205 °C. Because of the
geometry of sample, plane strain element is used to simulate the process. Current direction is from left to right. Also diffusion along boundaries is considered to be zero-blocking boundary condition. The displacement boundary conditions are assumed to be fixed at all boundaries, because both ends are connected through via for electrical connection and top and bottom boundaries are confined by passivated layers.

Before we proceed to compare our model simulation result with Valek’s experiment, a mesh sensitivity analysis is performed to show the robustness of our model. Two meshes are generated using ABAQUS CAE; A coarser mesh with 40 elements and a finer mesh with 180 elements; both elements are 8-node elements. The coordinates are set to be as \( x \) along length, \( y \) along thickness and \( z \) is along width. The meshes are shown on Fig. 1. The geometric dimension of the model is identical to Valek’s specimen.

Material properties used in analysis are listed in Table 1. For this comparison we use perfect

Table 1

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T ), temperature (K)</td>
<td>477 [21]</td>
</tr>
<tr>
<td>( k ), Boltzman’s constant (J/K)</td>
<td>( 1.38 \times 10^{-23} ) [9]</td>
</tr>
<tr>
<td>( E ) Young's modulus (GPa)</td>
<td>62 [19]</td>
</tr>
<tr>
<td>( \nu ), Poission ratio</td>
<td>0.33 [19]</td>
</tr>
<tr>
<td>Yield stress (MPa)</td>
<td>72 [19]</td>
</tr>
<tr>
<td>Equilibrium vacancy concentration</td>
<td>( 6.02 \times 10^{15} ) [27]</td>
</tr>
<tr>
<td>at a stress free state at 473 K (cm(^{-3}))</td>
<td></td>
</tr>
<tr>
<td>Atomic volume (cm(^{-3}))</td>
<td>( 1.66 \times 10^{-23} ) [9]</td>
</tr>
<tr>
<td>Vacancy relaxation time (s)</td>
<td>0.0018 [28]</td>
</tr>
<tr>
<td>( f ), average vacancy relaxation ratio</td>
<td>0.6 [28]</td>
</tr>
<tr>
<td>Effective charge number</td>
<td>4 [34]</td>
</tr>
<tr>
<td>Resisitivity (( \Omega )cm)</td>
<td>( 2.07 \times 10^{-7} ) [9]</td>
</tr>
</tbody>
</table>

Fig. 2. Results for coarser mesh after 24 h current stressing.
plasticity for aluminum material. So there are no hardening effects.

The computational results shown in Fig. 2 for coarser mesh are, respectively, normalized vacancy concentration, normalized atomic flux divergence, equivalent plastic strain and deviatoric stress distribution. Peak near the end is due to blocking boundary where transported flux is zero. Atomic flux divergence is calculated based on vacancy flux divergence and \( \frac{C_v}{C_a} = 1 \times 10^{-7} \) unchanged throughout the process. This term simply represents the percentage of mass transported out or in to the unit volume throughout the whole process. This variable is used to represent damage by many researches such as Sasagawa et al. [23].

Results shown in Fig. 2 indicate that without current crowding effects, atomic divergence still can happen because of the blocking boundary condition. Because of the discontinuity of vacancy flux at both ends, flux divergence and equivalent plastic strain distribution exhibit abrupt decrease near the boundary. Fig. 2 also shows that vacancy flux is on the same direction as current direction which will cause tension at right hand side (cathode) and compression at left side (anode), which is in accordance with Eq. (3). The counter diffusion caused by stress gradient and vacancy concentration is at the opposite direction of current direction. Plastic deformation takes place at two ends which propagates towards middle of line until reaching steady state.

The results for finer mesh are shown at Fig. 3. Compared with coarser mesh we can see finer mesh gives out same distribution as coarser mesh, maximum atomic flux divergence and deviatoric stresses for finer mesh result are very close to the values of coarser mesh.

4.2. Comparison with Valek’s experimental data

The experimental result reported by Valek [21] is shown below. The stress shown in Fig. 4 is deviatoric stress, where \( x \) is in the direction of the line, \( y \) is across the line, and \( z \) is normal to the sample surface. So Valek’s \( z \) direction is \( y \) direction in numerical analysis.
It should be pointed out that initial deviatoric stress must be considered during comparison. The experimental result report that maximum change in deviatoric stress along $x$ direction is 30 MPa, along $y$ direction is 35 MPa and along $z$ direction is 60 MPa. Valek calculates stresses as average value for grains [we believe] in the near right [or left] ends since they are maximum stress locations. Inspecting Fig. 3 we see that deviatoric stresses along $x$, $y$, $z$ direction are 30, 50 and 25 MPa, respectively, from numerical simulation. There is a good match between computational simulation and experimental data for deviatoric stresses.

In order to prove the necessity of plasticity in electromigration modeling, another simulation is performed using exactly same material properties and loading except this time we set yield stress to a much higher value, 200 GPa. Then we will have elastic mechanical response in the model. The simulation results are shown at Fig. 5. With elastic material properties, we predict a much higher stress near two ends which is almost three times bigger than experimental result.

After 24 h of current stressing, we set current to be zero for another 12 h. The simulation results shown at Fig. 6 compare vacancy distribution for finer mesh after 24 h and 36 h, respectively. The flux is as expected to flow on the opposite direction after we turned off the current. Fig. 7 depicts deviatoric stress distribution after 36 h. The stress relaxation is observed as expected.

To better illustrate the evolution of deviatoric stress and atomic flux divergence, an evolution history is given out completely for 36 h of analysis in Fig. 8. Here the data is collected from largest atomic flux divergence and equivalent plastic strain position, which is the second element from the left end of the mesh.
Fig. 8 clearly shows that plasticity has significant influence. From equivalent plastic strain and deviatoric stress history, we can see that after plastic deformation takes place, deviatoric stress will cease to grow which is in accordance with our perfectly plastic material properties. After turning off the current, three components of the deviatoric stresses decrease in accordance with Valek’s experiment. The most important feature of time evolution history of Fig. 8 is that both atomic flux divergence and equivalent plastic strain increase rate is much bigger after we increase the current. This is importance because atomic flux divergence and equivalent plastic strain are both very important features for material degradation. Both will contribute to nucleation and growth process of voids.

Fig. 7. Deviatoric stress distribution at 36 h (12 h after unloading).

Fig. 8. Stress, vacancy concentration, equivalent plastic strain and flux divergence evolution history.
4.3. Comparison with Korhonen’s model

In the thin film field, for its simplicity, Korhonen et al.’s [27] analytical model is widely used for one dimensional analysis. To prove effectiveness of our model, a simple analysis is performed to compare with Korhonen’s model. Wang et al. [35] performed an experiment on a 200 μm long and 0.5 μm aluminum thin film with a current density of $2.5 \times 10^4$ A/cm$^2$, Wang also derived an analytical solution using Korhonen’s model. The results of Wang’s experimental and analytical solution are shown in Fig. 9. Simulation results using the proposed model for Wang’s test are shown in Fig. 10. The results shown in Figs. 9 and 10 are spherical stress distribution along the specimen length. In Fig. 9 EM stress is spherical stress. From Fig. 10, we can see that the proposed model produce similar trend as Korhonen’s model as well as experimental result. Also at this current density, material is still in elastic range. It should be pointed out our tensile stress is positive while in Korhonen’s model, tensile stress is on negative sign. Because Wang did not give out units of stress in his paper, numerical comparison is not possible at this time. We realize that amplitude of the model simulation results for stresses are twice the data provided by Wang. Because Wang does not provide the units, a quantitative comparison is not possible. Yet qualitatively, simulation and experimental data are very similar. In the paper by Wang, he also mentioned that a stress localization behavior near 90 μm from cathode side, which he explained that may be caused by local microstructure irregularities. It is suggested by Wang that in order to simulate that locality effect, a local parameter which can represent initial defects should be included.

4.4. Comparison with Black’s data

Black’s [16] equation, which is the most commonly used mean time to failure equation (MTTF), gives out MTTF proportional to inverse square of current density. To illustrate relation between the current density with material degradation, several analysis are performed with the same condition as Valek’s experiment but with different current density values ranging from $1 \times 10^4$ A/cm$^2$ to $1 \times 10^6$ A/cm$^2$. The result is shown in Fig. 11. In Fig. 11, atomic divergence is divided into two separate graphs for different magnitudes of current density. With the smaller current density, there is no plastic deformation occurring. If we just take atomic flux divergence as a damage parameter
which is analogous to void ratio, then we can define a critical flux divergence as a failure criteria. Fig. 11 shows the limitation of Black’s equation. For lower current density it can never reach critical flux divergence no matter how long the current loading duration is. Also plasticity will have an effect on damage process when larger current density is applied which is not presented in Black’s formulation. This finding is also supported by Ye [36], his dissertation show that Black’s equation cannot be used to predict MTTF when temperature gradient, stress gradient or vacancy gradient are present.

5. Conclusions

A fully coupled diffusion-displacement analysis using inelastic mechanical material properties with regard to electromigration process is presented in this paper. The analysis yields good correlation between experimental and computational simulation results. The simulation results exhibit importance of inelastic mechanical behavior in electrical current loading which is neglected in the state of art research work, until very recently.

A very important finding of this paper is that it shows that Black’s MTTF equation is only valid for the test data and current range he used to come up with his model.

Another advantage of this model it is that it uses implicit formulation which is not limited by time step. In fact the time step larger than $\frac{\bar{E}}{D_{\text{effective}}}$ must be chosen to avoid oscillation of early results. This will decrease real time simulation computation time to a great extent. For a 2D problem in this paper, as shown above, it will take only a little of more than one hundred of increments to finish a
simulation for 36 h of real time and wall clock time consumed is on the order of minutes.

Third, the material integration scheme at each gauze point adopted return mapping method which is quadratic in convergence. That also speeded up the computation.

Finally, a fully coupled model is included to precisely illustrate interaction between diffusion field and displacement field.

Other features of this model include:

1. Accommodating of various current profiles.
2. Dealing with different geometry including 3D modeling.
3. Being able to incorporate various mechanical material properties, including most metals.
4. Being able to handle different boundary conditions, including displacement boundary conditions and flux boundary conditions.
5. The model enables us to simulate pre existing void inside a conductor material.
6. The model allows consideration of pre existing stress field influence.
7. The model utilizes widely used commercial software Abaqus with its strong modeling capability and powerful nonlinear solution solver.

The final goal of this model is to take the damage evolution model [25] into consideration, which is based on thermodynamic and continuum damage mechanics. The model can also be used to analyze solder alloy joints which are viscoplastic in nature.

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References


