Damage mechanics of electromigration in microelectronics copper interconnects

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Abstract: Current density levels are expected to increase by orders of magnitude in nanoelectronics. Electromigration which occur under high current density is the major concern for the nanoelectronics industry. Using a general purpose computational model, which is capable of simulating coupled electromigration and thermo-mechanical stress evolution, several dual damascene copper interconnect structures have been investigated for electromigration damage. Different diffusion boundary conditions including blocking and non-blocking boundary conditions, current crowding effects, interface diffusion effects and material plasticity have been considered. Different damage criteria are used for quantifying material degradation. The computational simulation results match the experimental findings; therefore the model proves to be a useful tool for quantifying damage in nanoelectronics interconnects.

Keywords: electromigration; copper interconnects; thin film; damage mechanics.


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1 Introduction

The reason copper has been chosen to replace aluminum for IC interconnects is its better resistance capacitance delay properties. Electromigration research on copper interconnects has increased during past several years. Compared with the research of aluminum electromigration, copper electromigration study is rather immature and its damage process is not understood as well as aluminum electromigration. The different material properties, integration techniques, and geometry of copper with aluminum thin films bring a new challenge to the investigation of copper electromigration damage.

A typical structure of aluminium and copper interconnects in a VLSI device is shown in Figure 1. The critical damage location (void nucleation) for aluminum is located at the upper edge of the left W via if the current flow is from left to right due to the blocking boundary condition provided by the W via. For copper interconnects, the critical point is at the bottom of the Cu via or the left upper edge of the Cu M2 layer if the current density is from left to right. The void nucleation at bottom of the via usually shows slit-like void nucleation according to Liniger et al. (2003), which represents an earlier failure mode. The void appearing at the upper edge of the Cu M2 layer is usually a large 3-D void and is sometimes combined with the slit-like void at its base. According to Liniger, this is the second mode of damage group when the blocking boundary condition is provided by the underlying Ta/TaN liner. This feature of multiple void nucleation may be the reason for the statistical multi-mode nature of the Median Time To Failure (MTF) of copper interconnects, while the MTF of aluminum interconnects is well represented by a single mode log normal distribution. Surface migration is considered in copper interconnects as a fast diffusion path. Different surface coatings will bring different MTF distributions (Hu et al., 2002) which show that surface migration might be an important factor in copper.

Figure 1  Cross section of a aluminum interconnect (top) and a copper interconnect (bottom)
The thickness of liner will also affect the failure time distribution. Different thicknesses of diffusion barrier liners (from 10 nm to no liner) have been used to investigate the effects (Liniger et al., 2003). When the liner thickness is less than 10 nm it first shows an increase in life time, but with further reduction (below 1.4 nm) the life time of the copper interconnects decreases. This is also reported by Hu et al. (2001). Studies reported above are largely experimental in nature. In this paper an electromigration-thermomigration model, developed at UB Electronic Packaging Laboratory, was utilised for computer simulation of these tests different boundary conditions are taken into account for the simulation presented in this paper.

Current distribution is also considered an important factor by Tu and Zeng (2002). Tu suggested that current crowding is the reason for void nucleation at the upper edge of the M2 layer where a very small current density exists. Tu and co-workers use current density gradient as a driving force to explain vacancy build up and void nucleation for sites with small current density. In this study, current density distribution is included in the investigation of damage, yet current density gradient is not considered as an additional field force.

In the literature usually copper is considered to be elastic during electromigration, in here material plasticity is used to examine the effect of that simplification.

2 Modelling and FEM implementation

The model used in this study has been published in previous papers published by Lin and Basaran (2005), Basaran et al. (2003) and Ye et al. (2003, 2004a, 2004b). Here, only a brief summary of the equations used are presented. The conservative equation for vacancy is

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

(1)

where \( C_{v0} \) is equilibrium vacancy concentration in the absence of a stress field, \( c \) is normalised vacancy concentration and \( c = \left( C_v / C_{v0} \right) \), \( C_v \) is vacancy concentration, \( t \) is time, \( q \) is vacancy flux and \( G \) is vacancy generation/annihilation rate.

Assuming that the driving forces of vacancy flux are also the vacancy concentration gradient, electrical field forces, stress gradient and thermal gradient, the vacancy flux is given by Sarychev and Zhinikov (1999) and Basaran et al. (2003):

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

(2)

where \( D_v \) is vacancy diffusivity, \( Z^* \) is vacancy effective charge number, \( e \) is electron charge, \( \rho \) is metal resistivity, \( \mathbf{j} \) 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 the spherical part of the stress tensor, \( \sigma_{\text{spherical}} = \text{trace} (\mathbf{\sigma})/3 \) and \( Q^* \) is the heat of transport, the isothermal heat transmitted by moving an 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 Sarychev and Zhinikov (1999):
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\[ G = -C_{\text{vo}} \frac{e - C_{ve}}{\tau_s} \]  

where

\[ C_{ve} = e^{\frac{(1-f)\Delta H_{\text{e-ph}}}{2T}} \]

is normalised thermodynamic equilibrium vacancy concentration. \( \tau_s \) is characteristic vacancy generation/annihilation time. The stress-strain constitutive model is established as:

\[ \sigma = C(e_{\text{total}} - e_{\text{plastic}} - e_{\text{electromigration}} - e_{\text{thermal}}) \]  

where \( C = \kappa \otimes I + 2\mu(1 - (1/3) I \otimes I) \) and \( \kappa \) is bulk modulus, \( \mu \) is shear modulus and

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

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

Itemised strain components:

\[ e_{\text{total}} = \frac{1}{3} e_{\text{trace}}^{\text{trace}} \times I + e_{\text{dev}}^{\text{dev}} \]  

\[ e_{\text{viscoplastic}} = \frac{1}{3} e_{\text{trace}}^{\text{trace}} \times I + e_{\text{dev}}^{\text{dev}} = e_{\text{viscoplastic}}^{\text{viscoplastic}} \]  

\[ e_{\text{electromigration}} = \frac{1}{3} e_{\text{trace}}^{\text{trace}} \times I + e_{\text{dev}}^{\text{dev}} = e_{\text{electromigration}}^{\text{electromigration}} \times I. \]

By substituting equations (5)–(7) into equation (4), we obtain

\[ \sigma = \kappa \times (e_{\text{trace}}^{\text{trace}} \times I + 2\mu(e_{\text{dev}}^{\text{dev}} - e_{\text{viscoplastic}}^{\text{viscoplastic}}) \]

where \( e_{\text{trace}}^{\text{electromigration}} \) is described by following equation

\[ \frac{\partial e_{\text{trace}}^{\text{electromigration}}}{\partial t} = \Omega C_{\text{vo}} (f \nabla q + f' \mathcal{G}) \]

\[ f' = 1 - f. \]

The finite element subroutines were coded based on above formulation and embedded into ABAQUS. A fully coupled scheme is used to simulate the stress and vacancy evolution.

Several methods are used to calculate the damage in copper interconnects. Total atomic flux divergence (integrated over time and local volume) is calculated according to the relationship between vacancy flux and atomic flux, which are equal to
each other. Local vacancy concentration and spherical stress values were also used as critical damage metric. Yield stress was also used as a critical value for damage simulations. These different damage criteria were compared and discussed in the following section.

3 Finite element modelling

8-nodesd higher order user defined elements were used to mesh the geometry. The length of the interconnect simulated varied from 50 µm to 300 µm. The interconnect thickness is 1 µm and the via height is 2 µm. The dimensions were chosen to simulate experimental data. The displacement boundary conditions considered are fixed along the copper interconnects. Different vacancy flux boundary conditions were considered for several cases. The mesh and boundary conditions (left and right edge) are shown in Figure 2. Six observation points are labelled in Figure 2 from a to f. These elements are potential sites for void nucleation. Also, a thin layer of Ta/TaN liner is modelled at the bottom of the via and above the left end of the copper interconnect. This is used to define the (diffusion) vacancy flux boundary condition. In the Ta/TaN layer, the outer surface is fixed at a vacancy concentration degree of freedom equal to the value of one, which is the initial normalised vacancy concentration at a stress free state. When a blocking boundary condition was considered, then the flux diffusivity of this layer was assumed to be 30 orders of magnitude smaller than the vacancy flux diffusivity in a copper grain boundary. Different diffusivity numbers generate various flux boundary conditions from non-blocking boundary conditions to fully blocking boundary conditions.

4 Determination of material properties

Material parameters are summarised in this section. Young’s modulus of copper is set to be 120 GPa and the Poisson’s ratio is set to 0.3. The ambient temperature is 473 K.
The following values of grain boundary and surface diffusivity are used based on work by Tu (2003) $D_{gb} = 1.2 \times 10^{-9}$ cm$^2$/s and $D_s = 1.0 \times 10^{-8}$ cm$^2$/s.

Ignoring the surface diffusivity (which will be taken into account later), the effective atomic diffusivity can be calculated as:

$$D_{at} = \frac{\delta D_{gb}}{d}$$

where $\delta$ (0.5 nm) is the grain boundary width and $d$ is average grain boundary diameter which is estimated to be 0.5 $\mu$m. Since in this formulation, vacancy diffusivity instead of atomic diffusivity is used, the relationship between vacancy flux and atomic flux is needed, to calculate effective vacancy diffusivity.

$$D_v C_a = D_v C_v$$

where $D_v$ is the effective atomic diffusivity, $C_a$ is atomic concentration.

The assumption of $(C_v/C_a) = 1 \times 10^{-7}$ is used. The effective vacancy diffusivity is calculated to be $1.2 \times 10^{-5}$ cm$^2$/s. The effective charge number $Z^*$ is 0.7 according to Ogawa et al. (2002). Other parameters are listed below:

- electric resistivity of copper is $1.6730 \mu\Omega$ s cm
- atomic volume is $1.1887 \times 10^{-11} \mu m^3$
- initial stress free state vacancy concentration is $8.413 \times 10^{15}$/ cm$^3$.

### 5 Current density distribution

In order to consider current density distribution, a separate electrical field analysis is simulated using ABAQUS. The current flow is from left to right. The current is considered to be uniform at the bottom of via with a magnitude of 4.5 mA/$\mu$m$^2$. Electrical potential at the right upper edge is set to 0. The current density is concentrated on the via-line corner as expected, which is shown in Figure 3. Also in Figure 3, two meshes are shown with the same current density load. The maximum current density in the finer mesh, which is of course at the corner of via-copper, is $16.36$ mA/$\mu$m$^2$. With coarser mesh the maximum density is $12.17$ mA/$\mu$m$^2$. The current density distribution along the line AB is shown in Figure 4. The figure shows that the current density distribution is mesh dependent around the corner. This is expected since the corner is a numerical singularity point and the analytical solution for current density is infinite at the corner. So if we want to utilise the current density distribution as our initial field input, we need to consider if the mesh dependence will affect the final solution. To investigate the latter, the current density distributions shown in Figure 3. Both were used as input for stress and vacancy coupled analysis with the same boundary conditions and material parameters. The results after 10 h of simulation, which are shown in Figure 5, show a small difference. Due to data processing difficulties, only the via and copper above the via are shown in Figure 5. This proves that the current singularity is localised and mesh dependence effect can be ignored for engineering purposes. Figure 5, exhibits that the spherical stress distribution corresponds to the current distribution and shows a turning point around the corner of the via-copper line.
Figure 3  Current density distribution

Figure 4  Current density distribution along line AB
5.1 Simulation case 1

A 50 µm long copper via is modelled. The copper film thickness is 1 µm. According to Hu et al. (1999), in such a thickness the diffusion path is a mixture of grain boundary and surface diffusion. In this case, pure grain boundary diffusion will be used. The mixture of diffusion paths will be considered in a later case. All the displacement boundary conditions are considered fixed. The flux boundary conditions are defined as blocking boundary conditions as stated in the previous part. Current loading is 45 mA/µm² and the flow of current is from left to right. The analysis was performed in two stages. The current density distribution is mapped as the initial field for the second stage displacement-vacancy coupled analysis. A fine mesh with typical element length of 0.125 µm will be used. The simulation was run for 100 h. Material plasticity is not considered.

The results at the six observation points (defined in Figure 2) are presented in Figure 6. Normalised vacancy concentration evolution in Figure 6(a) shows that inside the via or above the via the normalised vacancy concentrations are very close to each other. Points a and b are closest to the blocking boundary and are at the maximum vacancy concentration location. The same trend is shown in Figure 6(b) and (c) regarding spherical stress and total atomic flux divergence. Although the current density at point f is the highest, the vacancy concentration and flux divergence at point f is still smaller than at points a and b. Also at point d the current density is very small compared to the other points, but the vacancy concentration and flux divergence values are still very close to the values at other points. Current crowding is used by Tu et al. (2000) to explain the void formation at a no current region where point d is located. Based on our analysis results, we believe that the blocking boundary condition is the real reason for void nucleation in a no current region, because in our analysis we do not include the current density gradient as a driving force. Yet, we still observe vacancy build up at point d. Since vacancy flux is proportional to current density at the current concentration area, more vacancy will move out instead of moving in if there is current crowding. This is one source of vacancy flux divergence. Another source is the blocking boundary condition. The length of copper interconnect is much longer than the via height as a result, the blocking boundary conditions at right and at the bottom of the via are dominant compared
to the current density gradient. Thus, the vacancy concentration is mainly determined by the horizontal position of the points. Points a and b have relatively larger vacancy concentrations and flux divergences. This is because of the blocking boundary condition at the bottom of the via.

Figure 6  Time history of: (a) normalised vacancy concentration; (b) spherical stress; (c) total atomic flux divergence; (d) shear stress at six observation points; (e) vacancy flux at horizontal direction at middle of line and (f) shear stress distribution in via
Figure 6  Time history of: (a) normalised vacancy concentration; (b) spherical stress; (c) total atomic flux divergence; (d) shear stress at six observation points; (e) vacancy flux at horizontal direction at middle of line and (f) shear stress distribution in via (continued)
Figure 6  Time history of: (a) normalised vacancy concentration; (b) spherical stress; (c) total atomic flux divergence; (d) shear stress at six observation points; (e) vacancy flux at horizontal direction at middle of line and (f) shear stress distribution in via (continued)

In Figure 6(d) shear stresses at the six observation points are shown. Shear stress at points a and b is much larger than at the other points. This is caused by the interaction of volumetric strain at local points and the displacement boundary condition. Due to the vacancy build up at points a and b, the material will shrink. However, this shrinking is constrained by via-Ta/TaN interface since the Ta/TaN is a material with a much smaller vacancy diffusivity than bulk copper. Shear stress at points c and e is in the second place, and shear stress at points d and f is the minimum. Liniger et al. (2003) pointed out that under the blocking boundary condition, slit-like voids under the via are the major void type for early failure. Shear stress concentration located at the bottom of via in this simulation can explain the slit-like void nucleation in early failure observed by Liniger et al. (2003). Once the interface bonding strength or yield strength of copper is reached at the bottom of via, void nucleation at bottom of via onsets and propagates under the shear stress. This is the dominant mode of void nucleation. That is, the failure time is totally determined by void nucleation time. In a later case study, plasticity will be incorporated into the model. It will be shown that the time needed to reach the yield stress gives a prediction of failure time.

For points e and c, shear stress is much smaller than at the bottom of the via. In this region, the spherical stress is very high (tension stress is positive). Gleixner and Nix (1996) pointed out that at such high spherical stress, the void nucleation rate is still too slow to be responsible for void nucleation according to classical nucleation theory. In the Gleixner paper, an upper limit of 2 GPa of spherical stress is used. We can see from Figure 6(b) that spherical stress in this analysis is much smaller than 2 GPa. Gleixner pointed out that interface defect combined with high spherical stress may dramatically reduce the critical stress level for void nucleation. This can explain why large 3-D voids will appear in the upper surface of the copper lines where there is small current density. Since the shear stress level here is relatively low, void growth in this
region is totally determined by the flux divergence rate and is relatively slower than stress assisted void growth at the bottom of the via. This type of failure is described by Liniger et al. (2003) as the second mode of failure. Total atomic flux divergence in Figure 6(c) can be also considered an important damage criterion since it represents the decrease in atomic concentration level. In this analysis, since the steady state is reached, the change in atomic concentration level is relatively small.

In Figure 6(e), vacancy flux in the horizontal direction (which is the major flux direction) of an element at the middle point of the copper interconnect is shown. The flux reaches zero after 100 h of time which means that a steady state is reached. Figure 6(f) shows the shear stress distribution in the via and the copper interconnection above the via. The shear stress is concentrated at two sides of the bottom of the via. Since the current density distribution is assumed to be uniform at the bottom, the shear stress concentration at both corners of the interface is equal. In real interconnects, current density will be concentrated on the right corner if we take into account the M-1 layer in current field analysis. Thus, the right corner will be the most critical point.

5.2 Simulation case 2

To investigate different flux boundary conditions, the diffusivity in the Ta/TaN liner layer is set to one order of magnitude smaller than copper diffusivity. With the same current distribution input and the same displacement boundary condition as in case 1. Case 2 is also simulated for 100 h. The partial results at the observation points are shown in Figure 7. The spherical stresses are very small compared to the blocking boundary condition case. Also, the total atomic divergence and the shear stresses values are much smaller. This is expected since the flux divergence source in this simulation is controlled by the blocking boundary condition. At this boundary condition at the steady state, the total atomic flux divergence is reaching zero and the vacancy flux is at a very high level. MTF in this interconnect will be very long since there is a huge vacancy reservoir at the bottom of via. If we include a M-1 layer into the simulation, damage will focus on the M-1 layer since the vacancy source in the M-1 layer can not be infinite. The experimental results (Liniger et al., 2003) are in accordance with the simulation results presented in Figure 7.

Figure 7  Time history of: (a) spherical stress; (b) total atomic flux divergence and (c) shear stress at six observation points
5.3 Simulation case 3

The shear stress concentration is at the two corners of the via bottom (points a and b), the yield stress at these two points can be reached and plastic strain accumulation will further assist void nucleation. A plasticity model with yield stress of 69 MPa and no hardening is considered in this simulation case 3. Blocking boundary condition is also considered. Other material parameters are the same as with case 1. The simulation results are shown in Figure 8. Figure 8(a) shows the equivalent plastic strain accumulation evolution at the six observation points. Points a and b have the same plastic strain, and the other points...
have no plastic strain accumulation. The time reaching yield at points a and b is roughly 4.75 h. If the yield stress is defined as a damage metric, the time to failure was around 5 h during the simulations, which is in the same order of magnitude as the MTF of the first failure mode reported by Liniger et al. (2003). Spherical stress results are very close to case 1 which is shown in Figure 8(b). Figure 8(c) shows the shear stress distribution at the six observation points. For the other points, except points a and b, shear stress is very close to simulation case 1. For points a and b, shear stress level is much smaller than in case 1. After reaching the yield point, shear stress in points a and b decrease a little and finally reach a steady state. This decrease is due to stress relaxation with plastic strain in the local region. To study the influence of plastic strain on overall simulation results, normalised vacancy concentration and total atomic flux divergence are compared in Figure 9 for point a. These results are very close to each other, which show that the plastic strain does not have strong influence on the results.

Figure 8  Time history of: (a) equivalent plastic strain; (b) spherical stress and (c) shear stress at six observation points
Figure 8  Time history of: (a) equivalent plastic strain; (b) spherical stress and (c) shear stress at six observation points (continued)

Figure 9  Comparing between cases 1 and 3 in point: (a) total atomic flux divergence and (b) normalised vacancy concentration
5.4 Simulation case 4

A 300 µm long copper interconnect line is simulated in case 4. All the material parameters and boundary conditions are the same as in case 1 except the length of copper line. Results of the simulation are shown in Figure 10. Figure 10(a) shows the normalised vacancy concentration evolution history in the 100 h simulation. The six observation points’ normal vacancy concentrations are very close to each other in value, however, points a and b, have the largest vacancy concentration. Flux divergence and spherical stress results share the same trend. This further verifies that with longer length, horizontal direction vacancy flux is more dominant and current crowding effect in the via is very small. Shear stress distributions for the six observation points are shown in Figure 10(d). Shear stress in points a and b are much larger than in case 1. This is expected since the deformation caused by vacancy build up is much larger. Figure 10(e) shows the vacancy flux evolution and horizontal direction which is the major direction at the middle of the line. We can see from Figure 10(e) that a steady state is not reached.

Figure 10 Time history of: (a) normalised vacancy concentration; (b) spherical stress; (c) total atomic flux divergence; (d) shear stress at six observation points and (e) vacancy flux at horizontal direction at middle of line
Figure 10 Time history of: (a) normalised vacancy concentration; (b) spherical stress; (c) total atomic flux divergence; (d) shear stress at six observation points and (e) vacancy flux at horizontal direction at middle of line (continued)
A detailed comparison between cases 1 and 4 are shown in Figures 11 and 12. Figure 11 compares the shear stress and spherical stress evolution at point a. The shear stress and spherical stress of case 4 at point a are both much higher than in case 1. If we consider the plasticity in case 4, shear stress level will become almost the same for loading cases 1 and 4, but with larger plastic strain at case 4. The time to reach the yield point is controlled by shear stress, and from the results shown in Figure 11, the time needed to reach the yield stress for the longer line is the same as the shorter line. This is also verified by further analysis including the plastic strain for the longer line. Shear stress evolution comparison for point e is also shown in Figure 12. At point e shear stress is still very small even though vacancy concentration is much higher than in case 1. These results verified that a major source of shear stress is different diffusivity of the via and interconnect.

**Figure 11** (a) Shear stress and (b) spherical stress evolution for observation point a in cases 1 and 4.
According to the above analysis, with the longer interconnect length, time to reach critical shear stress at the bottom of via interface is the same for shorter interconnect line. The second failure mode which is the large 3-D voids at corner of the copper lines is much stronger than shorter lines since the vacancy concentration and flux divergence are much larger than in case 1. This trend is based on this analysis only and need to be further verified by experimental studies. It should be pointed out that current density at point d is very small and there is no current crowding gradient force applied at that point. Yet, vacancy concentration is very large.

5.5 Simulation case 5

The interface diffusion at the top surface of copper interconnect is considered a fast diffusion path by most researchers (Hu et al., 2002). To investigate this claim computationally, a fast diffusion path was created on the top surface of the copper interconnect. The diffusivity along this interface is set to be one order of magnitude larger than the vacancy diffusivity in the copper layer. All the other simulation parameters are the same as in case 1. The simulation results are shown in Figure 13. Figure 13(a) and (b) show the vacancy concentration and spherical stress for the six observation points. We can see that the fast diffusion path did not influence those six observation points’ evolution with respect to each other, although points d and e are much closer to the fast diffusion path. The shear stress distribution also shows the same pattern as the vacancy concentration and spherical stress. To further investigate this fast diffusion path, a two order of magnitude increase in interface diffusivity is used for another simulation case. The results are shown in Figure 14. Still there is no evidence of variation of response compared to case 1 for vacancy concentration, spherical stress or shear stress evolution. This can be explained by the dimension of copper interconnect thickness and the fact that the via is very small compared to the copper interconnect length. Although a fast diffusion path can favour those points which are close to it, this trend can not be distinguished since the distance between those six points are too small. The detailed comparison of point a in simulation case 1 and the two fast path simulation cases is shown in Figure 15. The evolution of normalised vacancy concentration, total atomic flux divergence, and shear stress are much faster with the fast diffusion path.
An experimental study by Hu et al. (2002) also showed that using a capping layer on the top of an interconnect surface can dramatically increase the MTF of a copper interconnect line.

**Figure 13** Time history of: (a) normalised vacancy concentration; (b) spherical stress and (c) shear stress at six observation points.
Figure 14  Time history of: (a) normalised vacancy concentration; (b) spherical stress and (c) shear stress at six observation points
Figure 15  Time history of: (a) normalised vacancy concentration; (b) shear stress and (c) total atomic flux divergence at observation point a.
6 Conclusions

Several simulation cases have been conducted in this paper. Based on the simulation results, two failure mechanisms are proposed. One is a shear stress controlled failure at the bottom of the via at the blocking boundary condition. The other is interfacial failure and void growth controlled failure at the end of a copper interconnect line. The increase in MTF through different capping layers may come from eliminating the fast diffusion path, strengthening the copper-capping layer interface, or both. Current density distribution is considered in this paper, and the analysis shows that the current crowding at the corner is not a major factor when compared with blocking boundary conditions. Also, material plasticity is considered and plastic strain accumulation is calculated. The stress relaxation after plasticity is also observed in this analysis. For non-blocking boundary conditions, the damage at the copper interconnect line is very small but vacancy flux is very large. The failure at the non-blocking boundary condition is controlled by mass depletion in other layer of copper interconnect lines.

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References


