

Electromigration Anisotropy and Mechanical Stress in Modern Copper Interconnect

H. Ceric^{1,2}, R. L. de Orio^{1,2}, and S. Selberherr²

¹Christian Doppler Laboratory for Reliability Issues in Microelectronics at the Institute for Microelectronics

²Institute for Microelectronics, TU Wien, Gußhausstraße 27-29, 1040 Wien, Austria

Phone: +43-1-58801-36032 Fax: +43-1- 58801-36099 Email: Ceric@iue.tuwien.ac.at

Abstract—Modern interconnect structures are exposed to high mechanical stresses during their operation. These stresses have their sources in interconnect process technology and electromigration. The mechanical properties of passivating films and the choice of process technology influence electromigration reliability. In this paper we analyze the interplay between electromigration and mechanical stress on an atomistic level. A stress-dependent diffusion tensor has been derived and implemented in a continuum electromigration model. Since the vacancy dynamics at grain boundaries also contributes to the stress distribution, the electromigration model has been extended by a grain boundary model. The plausibility of the compound model is demonstrated with an example of stress dependent electromigration in a three-dimensional, dual-damascene interconnect structure.

I. INTRODUCTION

There are three major sources of mechanical stress in passivated interconnect lines. The first one is the thermal stress, resulting from the difference in thermal expansion between the passivation and the metal upon cooling from high deposition temperatures. The second source of stress is the non-equilibrium film growth which is, as wafer curvature measurements have shown, even more significant than the thermal stress. The third major source of stress is electromigration itself.

Electromigration and stressmigration can increase local tensile stress or act against each other in order to reduce the tensile stress. The mechanical stresses generally change the local atomistic configuration which, in turn, causes an anisotropy of electromigration. The degradation process induced by anisotropic electromigration is far more difficult to predict than in the case of isotropic electromigration.

In this paper we introduce and discuss an atomistic electromigration model in which the anisotropy of material transport is induced by the anisotropy of the local stress field. The plausibility of the model is illustrated by a three-dimensional simulation.

The interplay between the local mechanical stress and electromigration on an atomistic level is studied in this work for the first time.

The introduced theoretical framework enables the study of anisotropic electromigration in the presence of different local

atomistic configurations in bulk, grain boundaries, and interfaces.

II. STRESS INDUCED ANISOTROPY OF ELECTROMIGRATION

Although the measurements significantly contribute to the understanding of thin film stresses, they are, in most cases, limited to simple test structures. Furthermore, the detailed stress distribution within a material cannot be experimentally determined.

The evolution of mechanical stress in interconnect lines depends on whether or not vacancies can be created or annihilated such that their equilibrium is maintained. For mechanical stresses to develop, there must be both a volume expansion or contraction of the line with respect to the surrounding material and a mechanical constraint applied by the surrounding material. As atoms exchange place with vacancies and travel towards the anode end of the line, there is a flow of vacancies towards the cathode end. In the absence of vacancy sources and sinks, this would result in a vacancy supersaturation on the cathode end and a deficiency at the anode end. Since the replacement of an atom with a vacant site produces a small relaxation in the surrounding lattice, there would be a net volume contraction at the cathode and expansion at the anode.

For the dual-damascene technology high tensile stress at the interfaces, where one can expect defects is critical. The conditions for electromigration and stressmigration can work both in order to increase this local tensile stress or act against each other in order to reduce the stress.

The choice of passivating film material and corresponding process technology causes tensile or compressive stress in the interface between the passivating film and the interconnect metal. Interfacial compressive stress diminishes electromigration along interfaces by reducing the diffusivity [1]. However, numerous experimental observations have shown [2] that tensile stress in the interface increases the possibility of failure.

Increased thickness and rigidity of the capping layer prevent relaxation of both thermal and electromigration induced stress, which results in dielectric cracking and metal extrusion.

As the analysis on the atomic level carried out by Schroeder and Dettman [3] has revealed, the vacancy flux J_v is separated in a diffusive part and a drift part

$$J_{v,i} = J_{v,i}^{\text{diff}} + J_{v,i}^{\text{drift}} = -\sum_j D_{ij}^v \frac{\partial C_v}{\partial x_j} - \frac{C_v}{kT} \sum_j D_{ij}^v \frac{\partial E_e}{\partial x_j}. \quad (1)$$

Instead of a scalar diffusivity (6), here we have a diffusivity tensor D_v with the components

$$D_{ij}^v = \frac{6D_0^v}{Z} \sum_{k=1}^Z a_i^k a_j^k \exp\left(-\frac{E_s^k - E_e}{kT}\right). \quad (2)$$

a_i^k are the normalized components of the jump vector \vec{r}_k (Fig. 1), and Z is the number of neighboring sites. D_0^v is the vacancy diffusivity in the ideal crystal lattice [4]

$$D_0^v = \frac{1}{12} Z \Gamma \lambda^2, \quad (3)$$

where λ is the vacancy jump length and Γ is the vibrational frequency of the crystal.

The application of a stress field σ generally causes a distortion of the saddle point energy E_s^k and the valley point energy E_e [3]. As one can see from (1), stress as a driving force acts only on the valley point energy E_e .

When a defect is created, the solid changes shape from its original condition (Fig. 2).

In linear elasticity theory, the change in the shape of a volume can be expressed with a real, symmetric tensor. For example, the distortion of a sphere into an ellipsoid produces a new volume Ω [5]

$$\Omega = \begin{bmatrix} \Omega_1 & & \\ & \Omega_2 & \\ & & \Omega_3 \end{bmatrix}.$$

Generally the symmetry of the shape change due to defect production depends on the symmetry of the defect.

The change of energy at the saddle point and the valley point is determined as an additional energy needed to create the defect in the presence of an external stress σ ,

$$E_s^k(\sigma) = E_s(0) + \Omega_s^k : \sigma, \quad (4)$$

$$E_e(\sigma) = E_e(0) + \Omega_e : \sigma, \quad (5)$$

where the stress is evaluated locally. $E_s^k(0)$ and $E_e(0)$ are the creation energies in the absence of external stresses. Ω_s^k and Ω_e are the changes in volume/shape imposed on the perfect, stressed crystal by placing the defect at the saddle point and the valley point, respectively. They are not equal to the creation and migration volumes.

The applied stress changes the energies at the saddle site and the valley site. The volume change caused by placing a vacancy at a valley site can be expressed as $\Omega_e = \Omega \epsilon_e^I$, where ϵ_e^I is the induced strain. In order to fully consider the influence of anisotropic stress on saddle site energies, the strain induced by placing a vacancy on the saddle point must depend on the jump direction \vec{a}_k , e.g. $\Omega \epsilon_s^I \cdot \vec{a}_k$ (Fig. 2), ϵ_s^I and ϵ_e^I are determined as

$$\epsilon_s^I = \begin{bmatrix} \epsilon_s & & \\ & \epsilon_s & \\ & & \epsilon_s \end{bmatrix}, \epsilon_e^I = \begin{bmatrix} \epsilon_e & & \\ & \epsilon_e & \\ & & \epsilon_e \end{bmatrix}, \quad (6)$$

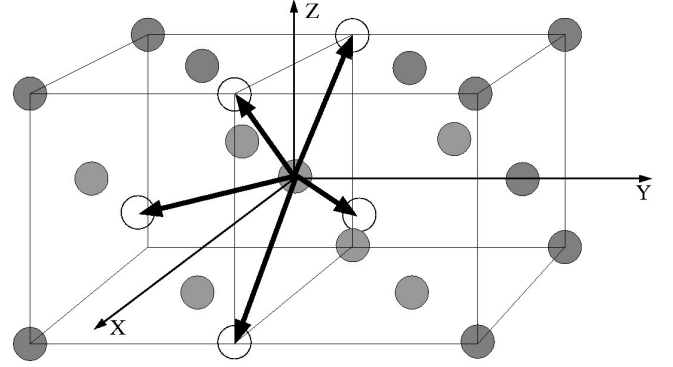


Fig. 1. Jump vectors in face-centered cubic (fcc) crystals.

since the vacancy exhibits at the valley as well as at the saddle site a cubic symmetry. Now (4) and (5) can be rewritten as

$$E_s^k(\sigma) = E_s(0) + \Omega(\epsilon_s^I \cdot \vec{a}_k) \cdot (\sigma \cdot \vec{a}_k) \quad (7)$$

$$E_e(\sigma) = E_e(0) + \Omega \text{tr}(\sigma) \epsilon_e, \quad (8)$$

By inserting these expressions into (2) one obtains

$$D_{ij}^v = \frac{6D_0^v}{Z} \exp\left(-\frac{E_s(0) - E_e(0)}{kT}\right) \exp\left(\frac{\Omega \text{tr}(\sigma) \epsilon_e}{kT}\right) \times \sum_{k=1}^Z a_i^k a_j^k \exp\left(-\frac{\Omega(\epsilon_s^I \cdot \vec{a}_k) \cdot (\sigma \cdot \vec{a}_k)}{kT}\right). \quad (9)$$

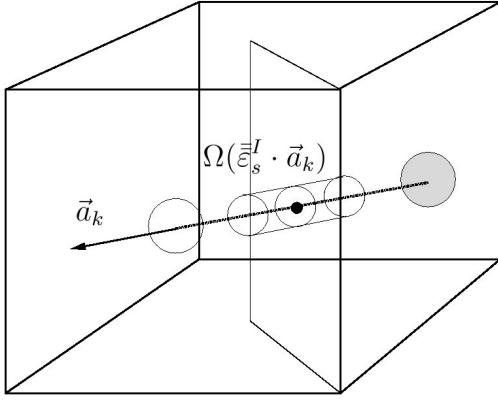


Fig. 2. Volume change caused by placing a vacancy at the saddle point in a stressed fcc crystal.

Then, equation (8) is set into (1)

$$J_{v,i} = -\sum_j D_{ij}^v \frac{\partial C_v}{\partial x_j} - \frac{C_v \Omega \epsilon_e}{kT} \sum_j D_{ij}^v \frac{\partial \text{tr}(\sigma)}{\partial x_j}. \quad (10)$$

The complete flux driven by stressmigration and electromigration written in vector form is now

$$\vec{j}_v = -D^v \left(\nabla C_v + \frac{C_v \Omega \epsilon_e}{kT} \nabla \text{tr}(\sigma) + |Z^*| e \nabla \varphi \right), \quad (11)$$

where φ is the electric potential which obeys Laplace's equation ($\Delta \varphi$) and Z^* is the effective vacancy charge.

Grain boundaries, as fast diffusion paths, play an important role in vacancy transport. They are capable of absorbing and emitting vacancies and thus they are also sites, where stress build up takes place. For an accurate description of the stress distribution inside an interconnect the physics of grain boundaries must also be taken into account. In [6] a model is introduced, where a grain boundary is treated as a separate medium with the capability of absorbing and releasing vacancies. In the present work this grain boundary model is also used for simulation.

III. SIMULATION RESULTS AND DISCUSSION

The impact of thermo-mechanical stress on electromigration induced vacancy transport is illustrated with a typical dual-damascene interconnect structure (Fig. 3). Generally, each portion of interconnect is embedded in a surrounding which has spatially varying mechanical properties.

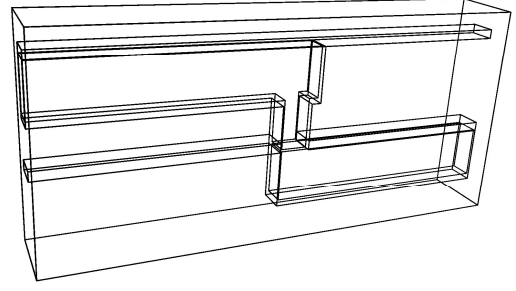


Fig. 3. Dual-damascene layout used. Top and bottom of the structure are mechanically fixed for thermomechanical simulation.

This is caused by the three-dimensional character of interconnect layouts as well as the different mechanical properties of materials used for dielectric, barrier, and capping layer. We have used the following parameters:

- Cu (interconnect): $Z^*=4$, $f=0.4$, $\Omega=1.182 \times 10^{-23} \text{ cm}^3$, $E=125 \text{ GPa}$, $\nu=0.34$;
- Ta (barrier): $E=380 \text{ GPa}$, $\nu=0.27$;
- Si_3Ni_4 (capping): $E=380 \text{ GPa}$, $\nu=0.27$;

The mechanical complexity of the interconnect's surrounding is modeled by setting appropriate mechanical boundary conditions (Fig. 4). The layout under consideration is bounded by a rectangular box (800 nm x 100 nm x 400 nm), the top and the bottom of the box are mechanically fixed (Fig. 4). Before starting an actual electromigration simulation a thermo-mechanical simulation is carried out. The layout is cooled down from 120°C to 20°C. Due to mismatch of the thermal expansion coefficients of the different materials a mechanical stress is built up. In Fig. 5, Fig. 6, and Fig. 7, the σ_{xx} , σ_{yy} , and σ_{zz} components of the thermal stress tensor are shown, respectively. As we can see, the stress is anisotropic and tensile. Due to the geometry and boundary conditions the area of high tensile stress (over 400 MPa in Fig. 5) is spread throughout the via.

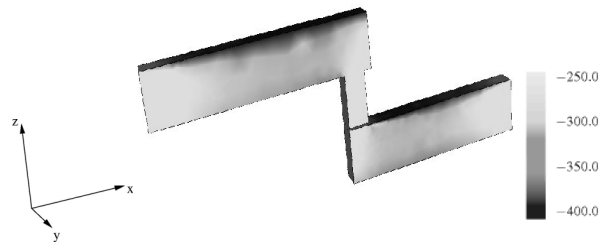


Fig. 5. σ_{xx} component of thermo-mechanical stress tensor [MPa].

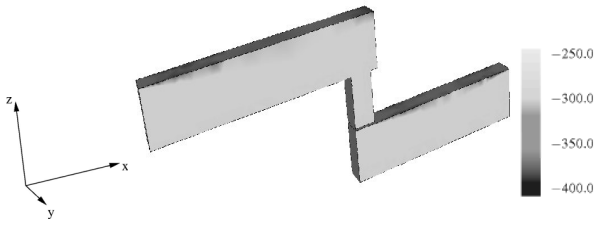


Fig. 6. σ_{yy} component of thermo-mechanical stress tensor [MPa].

Stress influences electromigration in two ways: it is an additional driving force and its presence is a source of anisotropy in diffusion.

The importance of stress as a driving force was early recognized and since then regularly included in electromigration models. However, from the atomic point of view, the effect of stress as a driving force can not be separated from the effect of crystal lattice distortion due to stress. In order to demonstrate the influence of stress, we compare the vacancy distribution modeled with a simple pressure dependent scalar diffusivity (Fig. 8) with one obtained considering stress dependent tensorial diffusivity (Fig. 9).

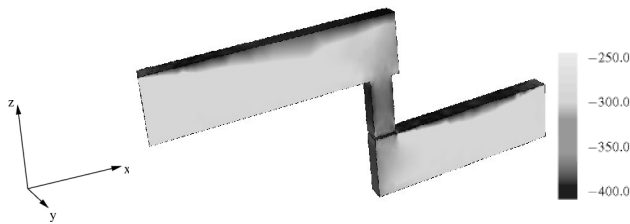


Fig. 7. σ_{zz} component of thermo-mechanical stress tensor [MPa].

In both cases we have simulated upstream electromigration with an applied current density of 8 MA/cm². It can clearly be seen in Fig. 9 that the anisotropic diffusivity causes a significantly more widespread area of high vacancy concentration (threshold of 5e16 cm⁻³) than in the case of scalar diffusivity. Wider areas of atom depletion are more probable to match weak adhesion spots at capping/interconnect interfaces and thus to induce void nucleation.

IV. CONCLUSION

A careful analysis of the connection between the local vacancy dynamics and stress build-up has been carried out. The obtained relations have been coupled to an electromigration model using the concepts of stress driven diffusion and anisotropy of the diffusivity tensor. The model presented in this paper is also based on a detailed analysis of the vacancy dynamics at the grain boundaries and the related mechanisms of stress build-up at triple points. A dual damascene architecture layout is used to illustrate and verify the introduced modeling approach.

Our simulations have shown that conditions for mass transport in lattice distorted by mechanical stress are significantly changed. Anisotropic stress causes a corresponding deformation of bulk lattice, which results in an anisotropy of the diffusivity. As a result we obtain a stress and vacancy distribution different from that, when only a scalar isotropic diffusivity is taken in account.

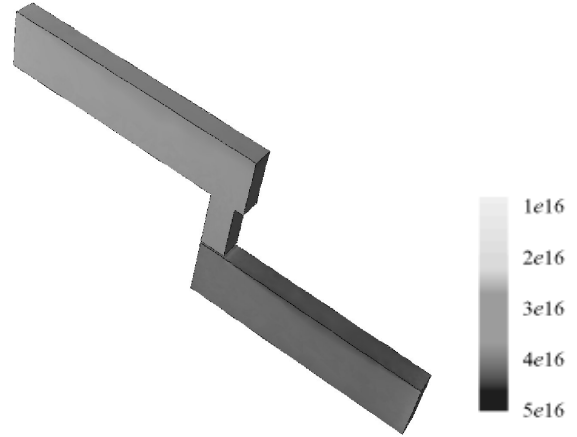


Fig. 8. Vacancy distribution after 10 min for the case of isotropic scalar diffusivity [cm⁻³].

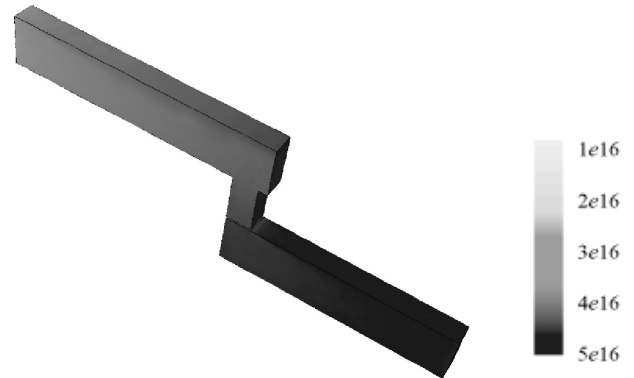


Fig. 9. Vacancy distribution after 10 min for the case of anisotropic tensorial diffusivity [cm⁻³].

REFERENCES

- [1] J. Lloyd and K. P. Rodbell, "Reliability," in *Handbook of Semiconductor Interconnection Technology*, edited by G.C. Schwartz and K. V. Srikrishnan, pp. 471–520, 2006.
- [2] J. Lloyd and J.J. Clement, "Electromigration in Copper Conductors," *Thin Solid Films*, vol. 262, no. 1, pp. 135–141, 1995.
- [3] K. Schroeder and K. Dettmann, "Diffusion Reactions in Long Range Potentials," *Z. Physik B*, vol. 22, pp. 343–350, 1975.
- [4] M. E. Glicksman, *Diffusion in Solids*. John Wiley and Sons, Inc., 2000.
- [5] M. S. Daw, W. Windl, N. N. Carlson, M. Laudon, and M. P. Masquelier, "Effect of Stress on Dopant and Defect Diffusion in Si: A General Treatment," *Phys. Rev. B*, vol. 64, p. 045205, 2001.
- [6] H. Ceric, R. L. de Orio, J. Cervenka, and S. Selberherr, "A Comprehensive TCAD Approach for Assessing Electromigration Reliability of Modern Interconnects," *IEEE Trans. Mat. Dev. Rel.*, vol. 9, no. 1, pp. 9–19, 2009.