Molecular Dynamics Simulation of Electromigration in Nano-sized Metal Lines

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The molecular dynamics simulation of electromigration has been made for nano-sized metal lines. By solving Laplace equations for the electric field using the relaxation method the current direction and the local current density were determined. In this model, a two-dimensional Lennard-Jones single crystal structure in contact with an insulator was first assumed. The periodic boundary conditions of both the current and atomic flows were setup in the direction of the applied voltage. The forces originated from atomic pair potential and electric field were setup to atoms in the molecular dynamics simulation. The simulations showed that the generations of vacancies, their movements and disappearances could be realized at the areas with a large current density. When the current direction was along the closest packing direction of atoms, the diffusion coefficient became largest. Results suggest an existence of thresholds of the voltage and temperature for the metal line lifetime.

keyword: electromigration, molecular dynamics simulation, metal line, electric field, diffusion, drift velocity

I. Introduction

Electromigration (EM), in which atom diffuses due to momentum received from electron has been studied since it causes disconnection and short circuit failure of metal lines in the integrated circuit and invites decrease in reliability. Statistical interpretation for the experimental results about the current density and the temperature dependencies of lifetime has been performed⁽¹⁾⁽²⁾. As line widths are larger than grain sizes, the dependencies of lifetime can be well explained by Black's rule⁽³⁾. It is known that when the line width is small lifetime becomes long and dispersive. However, this result is different from the expectation of Black's rule. This indicates that the influence of anisotropy and the grain boundary of crystal structure cannot be disregarded.

In the last decade, several computer simulations of electromigration in metal lines have been reported⁽⁴⁻⁹⁾ from the macroscopic viewpoint. However, as circuit integration shrinks to smaller dimensions, influences of crystal orientation and grain boundary structure on the lifetime must be taken into account. Recently, a simulation of the electromigration by molecular dynamics method

was proposed⁽¹⁰⁾, which paid attention to the mechanism of atomic diffusion. However, changes of current direction and density concerning with the void formation were not taken into consideration in the simulation, since the electric field was assumed to be uniform.

In this study, a molecular dynamics simulation of electromigration has been made for nano-sized metal lines. By solving Laplace equations for the electric field using the relaxation method the current direction and the local current density were determined. In this model, a two-dimensional metal single crystal structure in contact with an insulator was first assumed. In the calculation a Lennard-Jones atomic potential was used. The periodic boundary conditions of both the current and atomic flows were setup in the direction of the applied voltage. The atoms in the peripheries were treated as spices which keep their positions but influence inner atoms through interatomic potentials. In calculating the electric field, the periphery atoms were regarded as the insulating ones.

II. Simulation

In the molecular dynamics simulation of the electromigration, the force F_i originated from

electric field (F_e) and atomic pair potential (F_{LJ}) was applied to i atom as shown in the equation :

$$F_i = \sum_j F_{LJ}(r_{ij}) + F_e(x, y) \quad (1)$$

The molecular dynamics method calculates the change of the position, the velocity, and the acceleration by solving Newton's equation of each atom. The Lennard-Jones potential (eq.2) was used as a pair potential in this research

$$F_{LJ}(r) = 12\varepsilon \left(\frac{d^{12}}{r^{13}} - \frac{d^6}{r^7} \right) \quad (2)$$

where ε is the minimum energy and d the atomic radius.

A time step $dt = 0.005$ ps was used and the algorithm of Verlet was applied for the integration. For the calculation of electric field, the metal line was divided by many square meshes first and electric conductivity $\sigma(x, y)$ was regarded to be proportional to the existence probability of the atom around the lattice (x, y) using the Cloud In Cell (CIC) method. The electric conductivity $\sigma(x, y)$ is not uniform in our simulation. The electric potential $\phi(x, y)$ is shown in the Laplace equation :

$$\begin{aligned} & \text{div}[\sigma(x, y) \nabla \phi(x, y)] \\ &= \frac{\partial \sigma}{\partial x} \frac{\partial \phi}{\partial x} + \sigma \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial \sigma}{\partial y} \frac{\partial \phi}{\partial y} + \sigma \frac{\partial^2 \phi}{\partial y^2} \quad (3) \\ &= 0. \end{aligned}$$

The current is considered to be time independent since the flow of the electrons is much faster than the movement of the atoms. Metal line was simply regarded as a two-dimensional single crystal structure. In order to have nonuniform current in the metal line, the initial structure was designed to be two-dimensional single crystal which looks like "H" pattern as shown in Fig.1. After setting a voltage (Calculation was done under constant

Fig. 1 Two-dimensional single crystal structure and electron flow.

Fig. 2 Distribution of the electric potential $\phi(x, y)$ calculated by solving the Laplace equations.

voltage) at the electrode, the simultaneous equations were solved under the given boundary conditions at the peripheries of the medium and the voids in it. The electric potential $\phi(x, y)$ was obtained by the Gauss-Seidel method as well as the relaxation method. Fig.2 shows the electric potential distribution calculated on the basis of the two-dimensional model shown in Fig.1. By the gradient of the electric potential $\phi(x, y)$, the electric field $E(x, y)$ was determined (eq.4). Electron wind force $F_e(x, y)$ was assumed to be proportional to $E(x, y)$ (eq.5) and calculated on individual atom using the CIC method :

$$E(x, y) = -\nabla \phi(x, y) \quad (4)$$

$$\begin{aligned} F_e(x, y) &= Z^* e E(x, y) \quad (5) \\ &= \beta E_0(x, y) \\ &(\beta = Z^* e V). \end{aligned}$$

E_0 is the normalized electric field and V the applied voltage. Parameter β , which is proportional to the applied voltage, was set and changed since we did not know the value of effective charge $Z^* e$ (Z^* in a two-dimensional model is not able to correspond to actual parameter). The cooling operation to keep the temperature is necessary because the energy continues to accumulate due to applied voltage. The compulsive cooling was done at constant time intervals, so the rising temperature was reduced to a setting temperature.

The electromigration was simulated in a constant volume with fixed shell. Under the condition of constant pressure, it was necessary to determine the volumes (areas) of initial structures at different temperatures. In order to determine the volumes at temperatures from 0 K to 400 K, we used the constant pressure method proposed by Anderson⁽¹¹⁾.

Furthermore, in the simulation of electromigration, the periodic boundary conditions of both the current and atomic flows were setup in the direction of the applied voltage. The angle (α) between the closest packing plane and the direction of metal line (x -axis) was varied from 0 deg. to 30 deg. The periphery atoms were treated as insulator

Fig. 3 Successive simulated snapshots of electromigration at the condition of $\beta = 225$, Temp. = 10K. Small circles represent atoms in the metal line. Void formation process can be seen.

Fig. 4 Simulation of magnitude and direction of electron wind force corresponding to Fig. 3 (e-h).

atoms in the simulation and their sites were fixed.

The parameters of the Lennard-Jones pair potential and the calculation conditions are shown in Tables 1 and 2, respectively.

Table 1 Parameters of Lennard-Jones pair potential

atomic radius : d (nm)	0.24
ϵ / k (K)	120
atomic mass (Kg)	6.63×10^{-26}
number of atomic (atoms)	1050 ~ 1155
α (deg.)	0 ~ 30

Table 2 Condition for Simulation

Temperature (K)	10 ~ 200
Parameter for voltage : β (arb.unit)	200 ~ 400

III. Results and discussion

The successive simulated snapshots of a diffusion process in the case of $\alpha = 30$ deg. are shown in Fig. 3. As the drift velocity of the atoms becomes higher, the brightness of the atoms is increased. From the simulations, it is found that dislocations appear first and then vacancies form in the metal line near the anode as time passes by (a to d). As the atoms move towards the anode, the number of vacancies increases and void formation occurs in the metal line (e to h). The changes of electron wind forces are shown in Fig. 4, which corresponds to the process e to h in Fig. 3. Some regions in the metal line become thinner due to the void formation. The

Fig. 5 Drift velocity vs. applied voltage (β)

Fig. 6 Drift velocity vs. angle (α) between closest packing plane and x-axis

electron wind force becomes larger and its direction changes in these thinner places. In the case of $\alpha = 30$ deg., the voltage (β) dependencies of drift velocity at different temperatures are shown in Fig. 5. The drift velocity is slow as the voltage or temperature is low. Below 5 m/s, the drift velocity decreases rapidly as applied voltage is reduced. At that time atoms are vibrating and the formation of dislocation or vacancy is not found. When the drift velocity is higher than 5 m/s, it becomes proportional to the applied voltage. Atomic vibrations with large amplitudes introduce the formation of dislocations and vacancies. In the case of drift velocity over 10 m/s, the fast formation and successive movement of dislocation in the thin part of the metal line are observed in the simulation. Also, the formation of void does not happen at this stage due to fast diffusion of the atoms. As the temperature is 10K, the stable growth of void is observed only at the voltage range of 225 to 250 (arb. unit). It is suggested that the thresholds⁽⁶⁾⁽¹²⁾ of both of voltage and temperature affect the formation of dislocations.

The drift velocity at different voltage as a function of the angle (α) between the x-axis and closest packing plane is shown in Fig. 6. In the case of $\alpha = 0$ deg., dislocation appears between outer shell plane and next inner atomic plane, and the drift velocity is high though the voltage is low. The

drift velocity decreases as the angle (α) increases. This can be understood since the movement of dislocation is stopped at atomic step of restricted outer shell (the number of atomic steps increases as α increases).

IV. Conclusions

Simulation of electromigration was made by considering electric field, for which the electric potential was solved based on Gauss-Seidel method. The simulations showed that the generations of vacancies, their movements and disappearances could be realized at the areas with a large current density. When the current direction was along the closest packing direction of atoms, the diffusion coefficient became largest. Results suggest an existence of thresholds of the voltage and the temperature for the metal line lifetime.

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