

C-8-3

Development of Multi-Scale Electromigration Simulator Using Ultra Accelerated Quantum Chemical Molecular Dynamics and a Kinetic Monte Carlo Method and Its Application to Cu Interconnect

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1. Introduction

Electromigration(EM) phenomena typically appear in metallic interconnects and consist of the transport of metal atoms being driven by electron wind forces of high electric current density [1-3]. It is critical in many current devices since it is the most common mechanism of failure of the interconnections. Hitherto attempts to avoid its damaging effects involve, for instance, the addition of Cu to the Al material and adoption of Cu line systems. Despite these improvements, trends in micro-fabrication demand higher reliability. A large number of studies have been performed in this field including both the macroscopic prediction of line failure phenomenon under specific operation conditions [3,4], and the microscopic understanding of EM, which consists in the diffusion of metal atoms caused by electron wind forces[5], however few of these studies combine both the macroscopic and microscopic phenomena in order to achieve a better performing solution to the problem. Studies considering multi-scale simulations linking the device scale behavior with the atomic level dynamics are critical in the design of electronic devices.

In an attempt to bridge this gap we have developed two simulators for device scale simulation that uses a kinetic Monte Carlo (KMC) method to evaluate the lifetime of a connection line by formation of voids, together with an atomic scale simulator that can evaluate the probability for the KMC movement to a vacancy of a metal atom. The latter combines our originally developed electrical conductivity simulator [6] and ultra accelerated quantum chemical molecular dynamics (UA-QCMD) methods.

2. Methodology

The device scale EM simulation based on the KMC method was performed using a $4.56 \times 0.25 \times 0.27 \mu\text{m}$ model. This interconnect model was divided into 41,496 cubic

cells, each of $0.02 \mu\text{m}$ of edge length. A crystal grain area of 40 was set to compute the model. The probability of void movement was set to 100:1 at the grain boundary and the crystal grain respectively. The voids were generated at random positions on the model and were diffused according to the probabilities mentioned above using a KMC method simulator which has been newly developed in our laboratories. Analyzing the diffusion of voids enables the prediction of the interconnect failure.

Vacancy movement provability at the atomic level were predicted by an EM simulation scheme that was developed in the following way. First, the parameters for the tight binding quantum chemical molecular dynamics program (TB-QCMD) "Colors" were determined so as to reproduce the bond orders and the binding energies obtained by first-principle calculations. Electronic density distribution for the molecular orbitals that contribute to the electron conduction was obtained by "Colors" while the spatial distribution of the electron flow density was evaluated with an electric conductivity simulator also developed in our laboratories [6]. The UA-QCMD is achieved by updating the charges for the atoms of the simulated system and their binding energies during the molecular dynamics calculation. These values, obtained from a "Colors" calculation, are applied to the Morse and Coulombic terms of the potential energy. First-principles density functional code "DMol³" and "CASTEP" were used to verify the reliability of the parameters.

3. Results and discussions

In order to compare our results with experimental data for interconnects in a device, we used the device scale simulator. This simulator was designed according to the following specifications. Void cells are initially generated at random in the model. The moving direction of each void

cell is determined by the probability of movement of its neighboring cells which may belong to the grain boundary or the crystal grain regions. Void cells move to non void neighboring cells. In this simulation, an electric field of $3.4 \times 10^5 \text{ V/m}$, corresponding to a current density of $2.5 \times 10^{10} \text{ A/m}^2$, was applied. The results of the simulation are presented in Fig. 1. Here it can be observed that void cells tend to concentrate at one end of the interconnect, moving in the grain boundary along the direction of the electric field from an initial state of random dispersion. After 3,498 seconds of simulation the line failure is observed. This value corresponds fairly well to the experiment value [4].

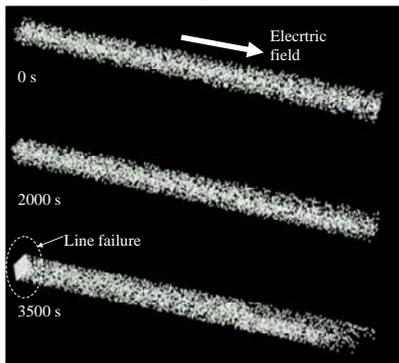


Fig. 1 Snapshots of device scale simulator (white points represents a void)

In order to correlate the probability of void movement with quantum chemical instances, for example activation energies, we also developed a simulator at the atomic level. In this simulator, tight binding parameters for the QCMD program “Colors”, namely data on ionization potentials in the solid and zeta parameters of Slater type atomic orbitals are firstly adjusted to reproduce the first principles calculation results of bond order, binding energy and charge for each type of orbitals. For this adjustment step a perfect crystal model consisting of 32 Cu atoms was used. The TB-QCMD calculation results using those parameters are shown in Table I. This table illustrates a good agreement of the “Colors” calculation with first principles results.

Table I The tight-binding quantum chemical molecular dynamics results using parameters obtained by first principles calculation

	Bond order between nearest atoms (-)	Binding energy (eV)	Charge (-)		
			s orbital	p orbital	d orbital
Tight-binding QCMD	0.18	90.7	0.52	0.78	9.71
First-principles calculation	0.2	76.7	0.53	0.83	9.64

To evaluate the spatial distribution of the electron flow density we used a cubic model constituted of 255 atoms and containing one vacancy. The data on the spatial distribution of singly occupied molecular orbitals were obtained by means of the “Colors”. After this step, the model was divided into $77 \times 77 \times 77$ cells and each of them was assigned the corresponding electron density data of the spatial distribution of the orbitals. Using this information, the spatial distribution of electron flow was computed by means of our

electrical conductivity simulator based on the KMC method. Furthermore, assuming that the electron wind force is proportional to the electron flow in each cell and is homogeneous within a cell, the spatial distribution of force by the electron wind can be established. The UA-QCMD simulation was executed under conditions 475 K of a temperature and $2.5 \times 10^{10} \text{ A/m}^2$ of current. Here the Morse type potential and the Coulombic potential were determined via the above mentioned scheme. The calculated trajectory of migration is shown in Fig. 2. Fig. 2 shows that the Cu atom closest to the vacancy moves to the vacancy position.

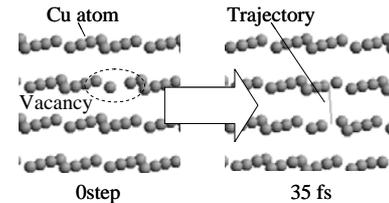


Fig. 2 Simulation results of atomic scale electromigration simulator

Finally, the mean square displacement of the moving atom with and without application of electron wind force is shown in Fig. 3. This figure shows that when an electron wind force is applied a Cu atom is displaced to the vacancy position, while when no wind force exist this displacement is not observed.

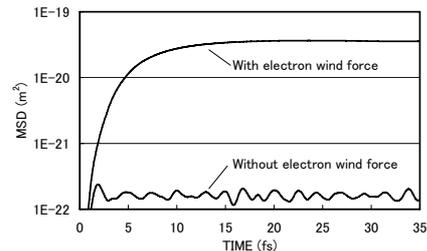


Fig. 3 Mean square displacement of the moving atom with electron wind force and the corresponding without electron wind force

4. Conclusion

We successfully developed new multi-scale EM simulators that are atomic and device level. Using these simulators, the prediction of lifetime for real scale interconnects based on atomic level knowledge has been available.

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