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Three Dimensional Molecular Dynamics Study of Void Electromigration in a Strained Bicrystal with a Grain Boundary

Shoso Shingubara, Taizo Fujii, Isao Utsunomiya, and Yasuhiro Horiike

Dept. of Electrical Engineering, Hiroshima University
Kagamiyama 1-4-1,Higashi-Hiroshima, 724, JAPAN

Stabilities and movements due to electromigration of a void in an Al lattice or in a bicrystal grain boundary are investigated by thrree-dimensional molecular dynamics simulations employing the empirical pair potential and the ballistic model for an electron wind force. It is shown that a void becomes more stable when a grain boundary energy increases. A void movement toward cathode direction, which is in good agreement with experiments, is simulated when a void is in the latice. However, the drift velocity of the void is significantly retarded when the void come close to the grain boundary. This may be due to the stabilaization effect of the grain boundary on the void.

1. INTRODUCTION

Metallic atom migration phenomena due to electric current (electromigration: EM) as well as thermal stress (stress-induced migration: SM) have been serious reliability problems in polycrystalline Al interconnections of ULSI. It is well known that differences in grain sizes and X-ray diffraction intensities of (111) orientation strongly influence reliability against EM and SM [1]. However, it has little been understood which kind of grain boundary a void is preferably formed, and what is more, how void growth, movement, and annihilation [2] occur due to EM and SM. The aim of the present study is to understand these phenomena from the atomistic point of view by a three dimensional molecular dynamics simulation.

2.MOLECULAR DYNAMICS MODEL

In our calculations, the atoms interact with each other through the empirical two body Morse potential [3]. The classical equation of motion for the atoms are solved by the Verlet algorism with a time step of 2×10^{-15} sec. The three dimensional simulation cells consisting of 800 to 1000 atoms are used. We consider different bicrystals; the one is (111) twin boundary with $\Sigma=7$ which consists of 6 atomic layers (Σ is an inverse of a number of coincident site lattice), and another is (001) twin boundary with $\Sigma=5$ which consists of 8 atomic layers (see Fig.1). For investigating EM, the classical ballistic model by Huntington and Grone [4] is used. The electron wind force F is expressed as $F=Z^*eE$, where we adopt the experimentally obtained value of Z^* [5]. Periodic boundary conditions are used at boundaries perpendicular to the current direction, and

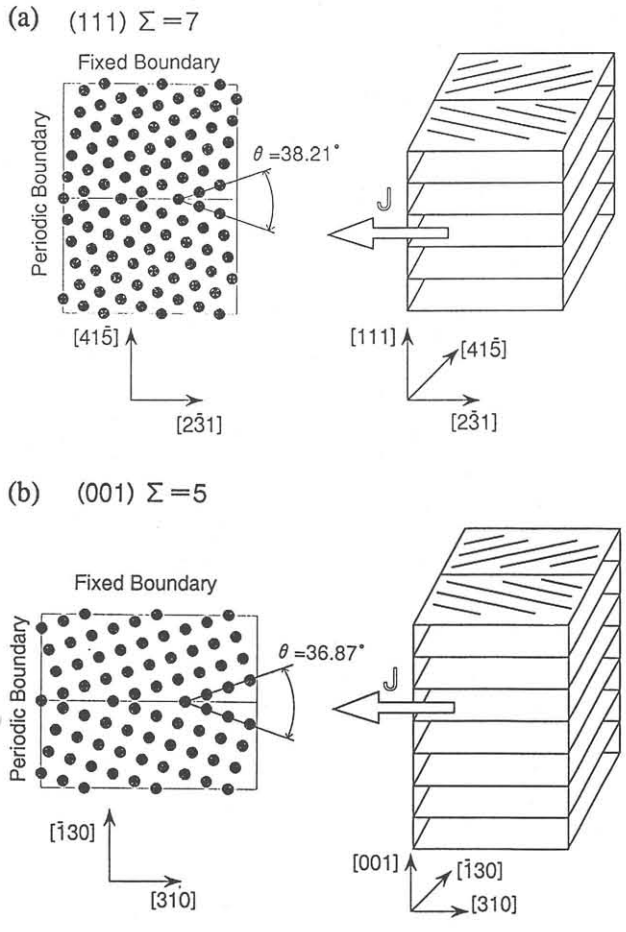

Fig.1 Schematic diagrams of computational cells.
(a) (111) twin boundary with $\Sigma=7$.
(b) (001) twin boundary with $\Sigma=5$.

boundaries at vertical directions (see Fig.1). Fixed boundaries are used for the both end parallel to the grain boundary. In order to incorporate an effect of equi-directional stress, a strain is introduced such that the fixed boundaries are uniformly stretched or compressed. Due to the limitation of the computational time, a simple model is adopted; for instance, a distribution of the current density is assumed to be uniform, and the electron wind force is introduced uniformly to every atom. Temperature is fixed constant during each run of calculation.

3.RESULTS AND DISCUSSIONS

At first, stability of a void in bicrystals which have different grain boundary structures is investigated as a function of a strain. Excess vacancies of 10% are initially introduced randomly in the lattice which is equi-directionally strained, then a stress relaxation occurs when time step proceeds. Relaxed structures of (111) twin boundaries with $\Sigma=7$, and (001) twin boundaries with $\Sigma=5$ are shown in Fig.2 and 3, respectively, for each case of 2% compression, no strain, and 2% tension. In the case of (111) boundary with $\Sigma=7$, a void is formed in every strain cases. However, a stable void is not formed when there is a 2% compressive strain in the case of (001) boundary with $\Sigma=5$. The results of stability of a void in various strain conditions are summarized in table 1. There is a tendency that a void becomes unstable when a compressive strain becomes large. It should be noted that the strain conditions where a void is stable is wider when Σ is larger. Calculated values of grain boundary energies for (111) boundary with $\Sigma=7$ is 0.43 [J/m^2], and that for (001) boundary with $\Sigma=5$ is 0.23 [J/m^2]. Thus, it is confirmed that a void is formed more easily in the grain boundary which has a higher grain boundary energy. Relaxation of the nearest neighbor atomic distance from the initial value is shown in Fig.4. It is evident that the amount of stress relaxation is large when a void is formed, and also it increases with the increase in grain boundary energy.

Secondly, the effect of EM on the behavior of a void is investigated for the (111) bicrystal with $\Sigma=7$ at the current density of 1×10^{10} A/cm^2 and 700K. Two cases of initial conditions are compared; the first case is that a void is in lattice and the grain boundary is normal to the current direction, and the second is that a void is on the grain boundary and the grain boundary is parallel to the current direction. The results of the first case is shown in Fig.5-a,b,c, and d. Void movement toward cathode direction is clearly observed in Fig.5-a,-b,and -c, which is qualitatively consistent with most of experimental observations [2,6] and the 2-dimensional simulation [7]. However, it seems that the drift velocity is retarded when the void come closely to the grain boundary as if the void is stabilized, as shown in Fig.5-

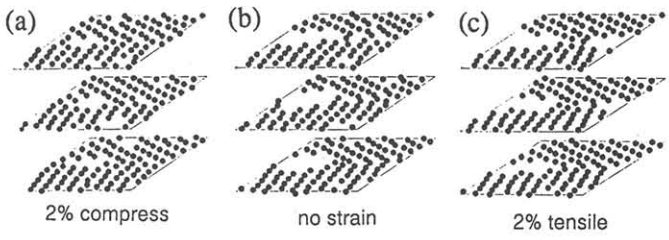

Fig.2 Stability of a void in an equi-directional strain in (111) bicrystal with $\Sigma=7$.
(a) 2% compressive strain, (b) no strain,
(c) 2% tensile strain, t=100 psec, 500 K.

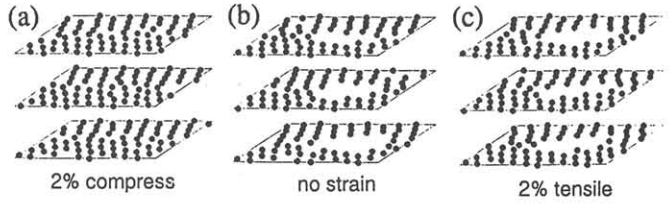

Fig.3 Stability of a void in an equi-directional strain in (001) bicrystal with $\Sigma=5$.
(a) 2% compressive strain, (b) no strain,
(c) 2% tensile strain, t=100 psec, 500 K.

grain boundary structure	compressive ← strain → tensile				
	4%	2%	0%	2%	4%
$\Sigma=1$	×	×	×	×	○
(001) $\Sigma=5$	×	×	○	○	○
(111) $\Sigma=7$	×	○	○	○	○

○ : stable, × : unstable

Table.1. Stability of the void under various strain conditions with and without the current stress.

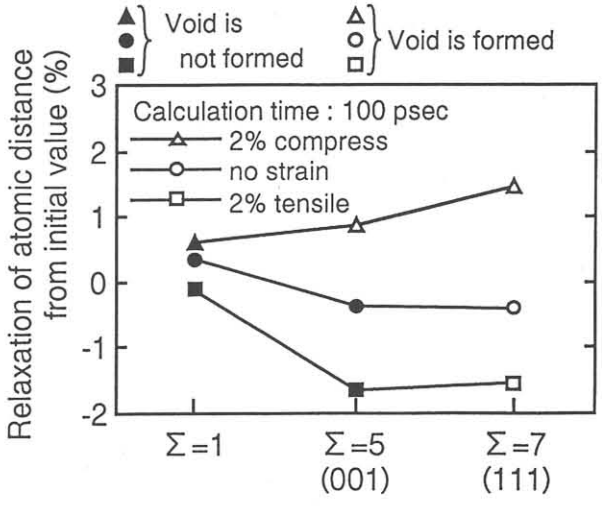

Fig.4 Relaxation of the nearest neighbor atomic distance from the initial value. t=100 psec, 500 K.

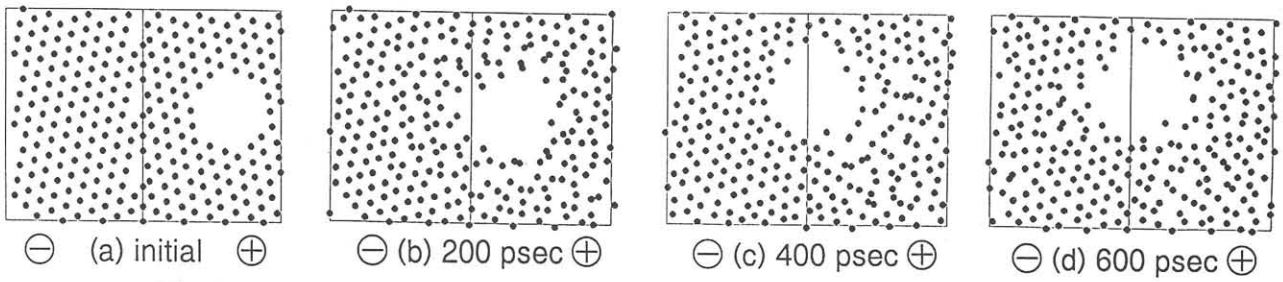

Fig.5 Void movement due to electromigration in the lattice. $1x10^{10}A/cm^2$, 700K.
(a) initial condition , (b) 200 psec, (c) 400psec, and (d) 600psec.

c to -d. Although this system is not thermal equilibrium, this behavior can be reasonably understood by assuming that the thermodynamics is approximately still valid. There are contributions of a grain boundary energy $A_{gb}\gamma_{gb}$, and void surface free energy $A_v\gamma_v$ in the Helmholtz free energy. When a void moves into the grain boundary from the lattice, the decrease of Helmholtz free energy occurs since there is a reduction of the grain boundary energy due to the shrincage of the grain boundary area. Whether this void penetrate through the grain boundary into the next grain or not has not been clarified yet, and a further simulation time will be needed.

On the other hand, the opposite result in the direction of the void movement was obtained in the second case (Fig.6-a,and b). A void initially situated at the grain boundary moved toward anode direction along the grain boundary. To the authors knowledge in the observations by in-situ SEM, there was a few cases of the void movement toward anode direction. These results can be understood as followings (see Fig.7). When the diffusion at the surface of the void is dominant, a void moves toward cathode direction since atoms at surface migrate toward anode direction. On the other hand, when the grain boundary diffusion is dominant, atoms come into the cathode side of the void and go out from the anode side, and consequently a void moves toward anode direction.

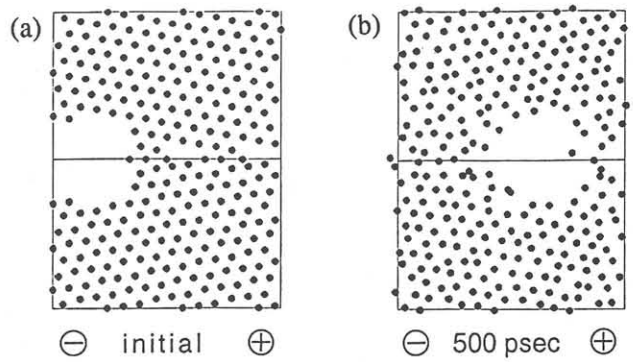

Fig.6 Void movement due to electromigration at the grain boundary. $1x10^{10}A/cm^2$, 700K.
(a) initial condition , (b) 500 psec.

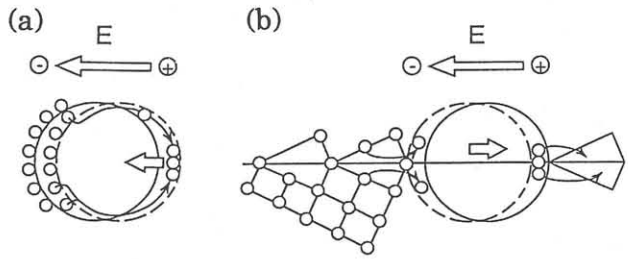

Fig.7 Illustration showing the atomistic view of the direction of the void movement. (a) surface diffusion, (b) grain boundary diffusion.

4.CONCLUSIONS

We succeeded in simulating the void movement due to electromigration by three-dimensional molecular dynamics. When a void is in lattice, void movement toward cathode direction is simulated, which is due to the surface migration. On the other hand, a void movement toward anode direction is simulated when a void moves along the grain boundary. It is considered that a grain boundary migration is dominant in the latter case. A significant retardation of a void drift velocity is found when a void come close to the grain boundary. This may relates to the so-called "the blocking effect" [8] of the atom migration flux in bamboo-like interconnects.

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