Molecular Dynamics Study of Impurity Effects on Grain Boundary Grooving*

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Impurity effects on grain boundary grooving in crystalline aluminum are studied using computer molecular-dynamics simulation. We use a Morse potential that includes equilibrium spacing (r_{Al}) and potential well depth ($|u_{Al}|$) to characterize aluminum/aluminum interaction, and a two-body interatomic potential that includes equilibrium spacing (r_m) and potential well depth ($|u_{min}|$) to characterize aluminum/impurity interaction. Simulations show that when r_m is smaller than r_{Al} and when $|u_{min}|$ is close to $|u_{Al}|$ (within $\pm 20\%$ of it), grain boundary grooving is prevented. This effect is explained by a decrease in the ratio of grain boundary diffusion to surface diffusion. Diffusion coefficients obtained in our simulations show that impurities at grain boundaries which satisfy the above conditions (e.g. copper) strengthen surface diffusion without strengthening grain boundary diffusion.

Key Words: Molecular Dynamics, Computational Mechanics, Diffusion, Grain Boundary Diffusion, Surface Diffusion

1. Introduction

Stress-induced voiding, which occurs even in the absence of electrical current, leads to deterioration in the reliability of metal interconnects in integrated circuits⁽¹⁾. As the metal line widths are expected to become smaller and smaller in the future, the problem of interconnect reliability will become more serious. Experiments^{(2),(3)} have shown that the addition of copper reduces the number of cracks and the failure rate in aluminum lines. In this paper we discuss what kinds of impurities could protect aluminum interconnects from voiding.

Grain boundary grooving is considered to play an important role in stress-induced voiding, because voids form at grain boundaries in metal lines. Therefore, although there are other void-causing factors

such as lattice diffusion and atom transport due to electrical current, we focus on grain boundary grooving. In particular, we will investigate the effects of impurities on grain boundary grooving using three-dimensional molecular-dynamics simulations.

Computer simulation techniques are useful in showing what kind of factors causes grain boundary grooving, because they make it easy to control such conditions as temperature and stress. Kitamura et al.⁽⁴⁾ have simulated grain boundary grooving by solving diffusion equations, and have found that groove profile is strongly dependent on the ratio of grain boundary diffusion to surface diffusion. They have also succeeded in demonstrating groove formation in two-dimensional molecular dynamics simulations⁽⁵⁾. Furthermore, they conducted a Monte Carlo simulation⁽⁶⁾ and obtained groove profiles similar to those obtained from their diffusion equations⁽⁴⁾.

As a result of these studies, properties of grain boundary grooving are now easier to understand. In a previous paper⁽⁷⁾, we extended the examination of grain boundary grooving by using three-dimensional molecular dynamics simulation. The simulation results showed that grain boundary grooves are more

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likely to form when temperature or tensile stress increases. We also found that the likelihood of groove formation depended mainly on the ratio of grain boundary diffusion to surface diffusion.

In this paper, we investigate the kinds of impurities that can prevent grain boundary grooving in crystalline aluminum, using three-dimensional molecular dynamics simulation. Here, we assume that aluminum/impurity interaction can be represented as a two-body central force interaction.

2. Model and Method for Simulation

2.1 Computation cell and coordinate system

In this paper we simulate grain boundary grooving in bicrystalline aluminum using three-dimensional molecular dynamics (MD). The computation cell used in our simulations is a bicrystal model with a $[001](310)\Sigma=5$ tilt grain boundary, as shown in Fig. 1. The coordinate system is shown in Fig. 1, where the positive z direction is in the $[001]$ direction. Periodic boundary conditions are applied in the x and z directions. Therefore, there are periodic grain boundaries in the x direction. The top surface is left free to move while the lower layer of atoms (below Border 1) is fixed (Fig. 1). The computation cell contains 928 aluminum atoms and two impurity atoms. At time step 1, these two impurity atoms are positioned at $(2\sqrt{10}a, 9\sqrt{10}a/4, a)$ and $(4\sqrt{10}a, 9\sqrt{10}a/4, a)$, at grain boundaries, where a is the lattice constant (Fig. 1). We also carried out simulations with impurity atoms positioned in the grain bodies, but we obtained smaller impurity effects than in the case in which the impurity atoms were at the grain boundaries, so we will describe only the latter case here.

To calculate local diffusion coefficients we divide the computation cell into Regions S, B, G, and C, as shown in Fig. 2 (L_x and L_y , the lengths of this cell in the x and y directions, are $4\sqrt{10}a$ and $3\sqrt{10}a$, respectively, where a is the lattice constant). Regions S, B,

Fig. 1 Computation cell and coordinate system

and G are used to represent surface, bulk, and the grain boundary, respectively. Region C represents the intersection of the grain boundary and the surface. The corresponding diffusion coefficients D_s , D_B , D_G , and D_C are calculated using Einstein's relation from the mean square displacements of the atoms in each region. The ratio, D_C/D_s , has been linked to the likelihood of groove formation⁽⁷⁾ (see section 3.1).

2.2 Calculation method

In this paper, we use two-body central force interactions to characterize interatomic potentials, and calculate atom positions by numerically solving Newton's equations of motion using the Verlet algorithm⁽⁸⁾. The basic time step increment is set at $h = 3.0 \times 10^{-15}$ s. We used the Morse-type potential from Ref. (9) to characterize the aluminum/aluminum (Al/Al) interaction. We also used two-body potentials (Appendix A), determined in Ref. (10), to characterize the impurity/impurity interactions for the seven kinds of impurities studied: Cu, Mg, Cr, Ni, Au, Zr, and Zn. Furthermore, we assume that Al/impurity interaction can be represented as the average of the Al/Al and impurity/impurity interactions. As an example, the Al/Cu interaction obtained from this assumption is shown in Fig. 3. This kind of Al/impurity interaction

Fig. 2 Regions C, S, G, and B

Fig. 3 Al/Al and Al/Cu potentials

is characterized mainly by potential well depth $|u_m|$, equilibrium spacing r_m , and curvature at minimum potential $k=d^2u/dr^2|_{r=r_m}$, as shown in Fig. 4. We pay attention only to $|u_m|$ and r_m because our simulations showed that neither k nor the atomic mass of the impurity has significant influence on the effects of the impurity on grain boundary grooving.

We investigate impurity effects not only from the seven real impurities described above (i.e., Cu, Mg, Cr, Ni, Au, Zr, and Zn) but also from other, theoretical impurities. We use the following Morse-type potential to characterize the interaction between an aluminum atom and a theoretical impurity atom.

$$u(r) = -u_{\min} \{ \exp[-2b(r-r_m)] - 2\exp[-b(r-r_m)] \} \quad (1)$$

The fifty-five pairs of u_m and r_m values (i.e. theoretical impurity types) shown in Fig. 5 were used in our simulations. In Fig. 5, impurities with identical r_m

Fig. 4 Interatomic potential

Fig. 5 u_m and r_m values for cases simulated

values are shown by identical symbols. The value of b in Eq. (1) was determined so that $k=2b^2|u_{\min}|$, the curvature at the minimum $u(r)$, equaled that for the Al/Al interaction. The masses of the theoretical impurity atoms were all set to be the same as that of an aluminum atom.

In a previous paper⁽⁷⁾, we found that grain boundary grooves are more likely to form when tensile stress increases. Therefore, we held the stress at zero during our simulations, to obtain the effects on grain boundary grooving caused only by impurities. This was done by controlling L_x and L_z , the lengths of the computation cell in the x and z directions. In addition, the temperature was controlled by a velocity-scaling method⁽¹¹⁾.

3. Simulation Results

3.1 Impurity effects at low temperature

Our simulation results showed that significant impurity effects were likely to be observed at low temperatures (below 650 K). We will discuss the difference in the magnitude of impurity effects between high and low temperatures later. In this section we will describe the impurity effects at low temperatures, based on our simulation results for $T=600$ K.

When no impurity is contained in the computation cell, a groove about 1 nm deep forms at the intersection of the grain boundary and the surface, that is, Region C of Fig. 2 (see Fig. 6). The depths of grain boundary grooves obtained by the simulations with impurities are shown in Fig. 7. The symbols by which the values of equilibrium spacing, r_m , are identified in Fig. 7 are the same as those in Fig. 5. Figure 7 shows that when r_m is smaller than $r_{Al}=0.2865$ nm and when $|u_{\min}|$ is close to $|u_{Al}|=0.0191$ aJ (within $\pm 20\%$ of it), grain boundary grooving is prevented. Here r_{Al} and $|u_{Al}|$ are the equilibrium spacing and potential well depth of the Al/Al interaction, respectively. Copper atoms, which satisfy the above two conditions, prevent grain boundary grooving, as shown in Fig. 8.

Fig. 6 Grain boundary grooving without impurities at $T=600$ K

Fig. 7 Depth of grain boundary grooves at $T=600$ K

Fig. 8 Grain boundary grooving with Cu atoms at $T=600$ K

Fig. 9 Grain boundary grooving with Mg atoms at $T=600$ K

This simulation result is consistent with experimental results^{(2),(3)}, which have shown that the addition of copper reduces the number of cracks and the failure rate in aluminum lines.

Magnesium atoms, which do not satisfy the condition $r_m < r_{Al}$, do not prevent grain boundary grooving, despite the fact that they satisfy the other condition that $|u_{min}|$ is close to $|u_{Al}|$ (Fig. 9). Furthermore, Cr atoms, which do not satisfy the latter condition, promote grain boundary grooving rather than preventing

Fig. 10 Grain boundary grooving with Cr atoms at $T=600$ K

Fig. 11 Relation between u_{min} and D_s at $T=600$ K

it, even though they satisfy the former condition that r_m is smaller than r_{Al} (Fig. 10).

We will now explain these impurity effects using the diffusion coefficients D_c and D_s for Regions C and S, respectively. The grain boundary groove is likely to form when atom migration from Region C into Region S is stronger than that from Region S into Region C. We assume that the magnitude of atom migration from Region C into Region S is represented by D_c , and that the migration from Region S into Region C is represented by D_s . Thus the groove becomes deep when the ratio D_c/D_s increases. This tendency was observed in simulations for models with no impurities in a previous paper⁽⁷⁾.

The diffusion coefficients D_s and D_c obtained by the simulations with impurity atoms are shown in Figs. 11 and 12, respectively. First of all, we will focus on the simulations in which $|u_{min}|$ was close to $|u_{Al}|=0.0191$ aJ. The D_s values for $r_m < r_{Al}$, which are represented by $\bullet$ and $\blacksquare$ in Fig. 11, are significantly larger than those for $r_m \approx r_{Al}$, which are represented by $\triangle$, $\times$, and $\blacktriangle$. On the other hand, the D_c values for $r_m < r_{Al}$ are nearly equal to those for $r_m \approx r_{Al}$ in Fig. 12. Thus D_c/D_s and groove depth for $r_m < r_{Al}$ are smaller than those for $r_m \approx r_{Al}$. The values of both D_s and D_c for $r_m > r_{Al}$ are significantly larger than those for $r_m \approx r_{Al}$ (Figs. 11 and 12). However, the values of D_c/D_s for $r_m > r_{Al}$ are not significantly different from those for $r_m \approx r_{Al}$. Thus, grain boundary grooving is not prevented

Fig. 12 Relation between $u_{\min}$ and D_c at $T=600$ K

Fig. 13 Grain boundary grooving with Cu atoms at $T=700$ K

Fig. 14 Relation between temperature and diffusion coefficients

when $r_m > r_{Al}$. Secondly, when $|u_{\min}|$ is not close to $|u_{Al}|$, the D_c values are much larger than the D_s values (Figs. 11 and 12), and therefore, the values of D_c/D_s and the groove depth are larger than for $|u_{\min}| \approx |u_{Al}|$. The effects of the impurities are thus explained by the decrease or increase in the ratio D_c/D_s . We will discuss the details of the mechanism by which impurities affect groove formation in section 4.1.

3.2 Grain boundary grooving at high temperatures

In this section we discuss the grain boundary grooving and impurity effects at high temperatures (above 650 K). Simulation results showed that a deep groove forms at such temperatures, despite the presence of Cu atoms, which prevent grain boundary grooving at lower temperatures (Fig. 8). For example, Fig. 13 shows a deep groove obtained in a simulation with Cu atoms at 700 K. Using the temperature dependence of the diffusion coefficients D_s and D_c we can explain why Cu atoms lose their groove-prevention effect at temperatures above 650 K. Figure 14 shows the relations between temperature and diffusion coefficients, obtained by simulation. As shown in this figure, D_c increases more rapidly with temperature than D_s even when Cu atoms are present. When the temperature increases, the ratio D_c/D_s becomes larger. For example, the D_c/D_s values with Cu atoms for 600 K and 700 K are 0.56 and 1.41, respectively (Fig. 14). Therefore, the deep groove forms at high temperatures even when there are Cu atoms present.

The slopes of the lines in Fig. 14 represent activation energies. The activation energies Q_c and Q_s (from D_c and D_s , respectively) are obtained from Fig. 14 as $Q_c = 3.8 \times 10^{-20}$ J and $Q_s = 0.78 \times 10^{-20}$ J. These values are almost independent of the presence of Cu atoms, as shown.

4. Discussions

4.1 Impurity effects on diffusion coefficients

Our simulations showed that when r_m is smaller than r_{Al} and when $|u_{\min}|$ is close to $|u_{Al}|$, grain boundary grooving is prevented. In section 3.1 this groove-prevention effect was explained as an increase in D_s with no increase in D_c . In this section we further discuss why impurities which satisfy above conditions *cause* this increase in D_s with no increase in D_c . We will investigate the impurity effects on the diffusion coefficients D_s and D_c by calculating the potential energy and mean interatomic distance. When the potential energy in a region is great, the atomic configuration is considered to be disordered and the atoms to actively move around. Furthermore, when the mean interatomic distance is large, diffusion is active. Because of these two facts, we can evaluate

the diffusion coefficient in a region on the basis of the potential energy and mean interatomic distance in the region.

We define the potential energy for Regions C and S (Fig. 2) as U_c and U_s , respectively. We also define the mean interatomic distance between nearest-neighbor atoms in Regions C and S as d_c and d_s , respectively. The values of U_c , U_s , d_c , and d_s obtained from our simulations at 600 K are shown in Figs. 15, 16, 17, and 18, respectively.

First, we will focus on the simulation cases in which $|u_{\min}|$ was close to $|u_{\text{Al}}|$. As shown in Figs. 15

Fig. 15 U_c obtained from MD simulations with $T=600$ K

Fig. 16 U_s obtained from MD simulations with $T=600$ K

Fig. 17 d_c obtained from MD simulations with $T=600$ K

and 16, the values of both U_c and U_s for $r_m < r_{\text{Al}}$ (symbols $\bullet$ and $\blacksquare$) are greater than those for $r_m \approx r_{\text{Al}}$ (symbols $\triangle$, $\times$, and $\blacktriangle$). This means that impurity atoms whose atomic radii are significantly smaller than that of an Al atom cause disorder in atomic configuration in Regions C and S. The d_c values for $r_m < r_{\text{Al}}$ are smaller than those for $r_m \approx r_{\text{Al}}$, as shown in Fig. 17. This means that impurity atoms whose atomic radii are significantly smaller than that of an Al atom attract other nearby atoms in Region C. The greater U_c values have a tendency to make D_c larger, while the smaller d_c values have a tendency to make D_c smaller. For $r_m < r_{\text{Al}}$, these opposite effects on D_c by the greater U_c and smaller d_c values cancel each other out, and the D_c values are therefore almost the same as those for $r_m \approx r_{\text{Al}}$ (Fig. 12). On the other hand, the d_s values do not depend strongly on the r_m values, as shown in Fig. 18. This means that impurity atoms which are located far from Region S hardly influence the d_s values at all. Thus the effect on D_s by the greater U_s values for $r_m < r_{\text{Al}}$ is not cancelled out by an opposite effect, and therefore makes D_s values larger than for $r_m \approx r_{\text{Al}}$ (Fig. 11). As a result of these effects, impurities which satisfy the conditions $r_m < r_{\text{Al}}$ and $|u_{\min}| \approx |u_{\text{Al}}|$ cause an increase in D_s with no increase in D_c , and therefore prevent grain boundary grooving.

When $|u_{\min}|$ is not close to $|u_{\text{Al}}|$, the U_c values are much greater than for $|u_{\min}| \approx |u_{\text{Al}}|$ (Fig. 15). The effect on D_c of the greater U_c values is so large that it is not cancelled out by the opposing effect due to smaller d_c values, so the D_c and D_c/D_s values are large enough for a deep groove to form even when $r_m < r_{\text{Al}}$. The same sort of thing happens at high temperatures (above 650 K). As shown in Fig. 14, D_c rapidly increases with the temperature, even when Cu atoms are present, due to rapid increase in U_c . Therefore grain boundary grooving is not prevented when the temperature is above 650 K, as we found in section 3.2.

Fig. 18 d_s obtained from MD simulations with $T=600$ K

When the atomic radius of the impurity is significantly larger than that of Al (that is $r_m > r_{Al}$), both the greater U_c (Fig. 15) and larger d_c (Fig. 17) make the D_c values larger than those for $r_m \approx r_{Al}$ (Fig. 12). In this case, therefore, D_c/D_s values are large enough for a deep groove to form even though the D_s values are also larger than those for $r_m \approx r_{Al}$ (Fig. 11).

Among the seven kinds of real impurities, Cu, Mg, Cr, Ni, Au, Zr, and Zn, we did not find any other than Cu that satisfied the conditions, $r_m < r_{Al}$ and $|u_{min}| \approx |u_{Al}|$. However, the results of this paper will be useful in searching for groove-preventing impurities when accurate interatomic interactions between various kinds of atoms have been obtained in the future.

4.2 Boundary conditions and temperature-controlling method

In our simulations periodic boundary conditions were applied in the x and z directions. Therefore, grain boundaries are positioned periodically in the x direction, and there are two grain boundaries in the computation cell in Fig. 1. One of these is in the center of this cell, and the other is on the side. There are thus two possible positions where a grain boundary groove might form. In the simulations, however, we made the groove more likely to form at the center grain boundary than the side one by using a center-first heating-control method. For example, when we wanted to set the temperature at 600 K over the entire computation cell, we first applied 600 K to Region C, with the temperature in the other regions kept at 300 K. Then, after a number of steps, we set the other regions to 600 K, as well. As a result, a groove was more likely to form in Region C than elsewhere.

5. Conclusions

Grain boundary grooving in crystalline aluminum was studied using molecular dynamics simulation, and impurity effects were investigated. We used a Morse-type potential that includes equilibrium spacing (r_{Al}) and potential well depth ($|u_{Al}|$) to characterize Al/Al interaction. We also used a two-body interatomic potential that includes equilibrium spacing (r_m) and potential well depth ($|u_{min}|$) to characterize Al/impurity interaction. The following results were obtained.

(1) Impurities which satisfy the conditions $r_m < r_{Al}$ and $|u_{min}| \approx |u_{Al}|$ prevent grain boundary grooving.

(2) Copper atoms, which satisfy the conditions described in (1), prevent grain boundary grooving at low temperatures below 650 K. This result is consistent with experiments.

(3) This groove-prevention effect is explained by the decrease in the ratio of grain boundary diffusion to surface diffusion. Diffusion coefficients obtained by

simulation show that impurities which satisfy the conditions described in (1) strengthen surface diffusion (D_s) without strengthening grain boundary diffusion (D_c) at the intersection of the grain boundary with the surface.

(4) When the temperature is above 650 K, grain boundary diffusion D_c is so large that grain boundary grooving is not prevented even when Cu atoms are present.

Appendix A. Interatomic potentials

The interatomic potentials^{(9),(10)} between atoms of the same element for the materials used in this paper are shown in Tables 1–8. Al/impurity interactions were obtained as the average of the Al/Al and impurity/impurity interactions. In Tables 1–8, r represents interatomic distance and the units of length and energy are nm and aJ (i.e. 10^{-18} J), respectively.

Table 1 Al/Al potential

$$u_{Al/Al}(r) = -u_{Al}\{\exp[-2b_{Al}(r-r_{Al})] - 2\exp[-b_{Al}(r-r_{Al})]\}$$

$$u_{Al} = -0.0191149 \text{ aJ}$$

$$b_{Al} = 23.53643 \text{ nm}^{-1}$$

$$r_{Al} = 0.2864944 \text{ nm}$$

Table 2 Cu/Cu potential

$$u_{Cu/Cu}(r) = -u_{Cu}\{\exp[-2b_{Cu}(r-r_{Cu})] - 2\exp[-b_{Cu}(r-r_{Cu})]\}$$

$$u_{Cu} = -0.0288382 \text{ aJ}$$

$$b_{Cu} = 23.27429 \text{ nm}^{-1}$$

$$r_{Cu} = 0.257063 \text{ nm}$$

Table 3 Au/Au potential

$$u_{Au/Au}(r) = -u_{Au}\{\exp[-2b_{Au}(r-r_{Au})] - 2\exp[-b_{Au}(r-r_{Au})]\}$$

$$u_{Au} = -0.0253176 \text{ aJ}$$

$$b_{Au} = 28.40901 \text{ nm}^{-1}$$

$$r_{Au} = 0.2882197 \text{ nm}$$

Table 4 Zr/Zr potential

$$u_{Zr/Zr}(r) = -u_{Zr}\{(r_{Zr}/r)^{12} - 2(r_{Zr}/r)^6\}$$

$$u_{Zr} = -0.0293670 \text{ aJ}$$

$$r_{Zr} = 0.317 \text{ nm}$$

Table 5 Zn/Zn potential

$$u_{Zn/Zn}(r) = -u_{Zn}\{(r_{Zn}/r)^{12} - 2(r_{Zn}/r)^6\}$$

$$u_{Zn} = -0.00955967 \text{ aJ}$$

$$r_{Zn} = 0.266 \text{ nm}$$

Table 6 Mg/Mg potential

Range	Potential
$r \leq 0.353034 \text{ nm}$	$-28.843 r^3 + 33.2763 r^2$ $-12.4159 r + 1.4893$
$0.353034 \leq r \leq 0.417222$	$-46.389 r^3 + 51.8577 r^2$ $-18.9751 r + 2.26112$
$0.417222 \leq r \leq 0.48141$	$60.8580 r^3 - 82.3412 r^2$ $+36.9993 r - 5.52120$
$0.48141 \leq r \leq 0.513504$	$-124.847 r^3 + 185.799 r^2$ $-92.0566 r + 15.1837$
$0.513504 \leq r$	0

Table 7 Cr/Cr potential

Range	Potential
$r \leq 0.2685 \text{ nm}$	$344476.1 r^5 - 385510.53 r^4$ $+167781.67 r^3 - 35083.543 r^2$ $+3450.3221 r - 122.00353$
$0.2685 \leq r \leq 0.3474$	$44186.012 r^5 - 70405.307 r^4$ $+44547.708 r^3 - 13991.919 r^2$ $+2182.5604 r - 135.38817$
$0.3474 \leq r \leq 0.4421$	$-36.364067 r^4 + 183.83738 r^3$ $-185.80852 r^2 + 69.065196 r$ -8.7131314
$0.4421 \leq r$	0

Table 8 Ni/Ni potential

Range	Potential
$r \leq 0.3008 \text{ nm}$	$-1587641.7 r^6 + 2167423.8 r^5$ $-1201163.5 r^4 + 342430.63 r^3$ $-52002.109 r^2 + 3837.9981 r$ -96.8624
$0.3008 \leq r$	0

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