Modeling Nucleation and Growth of Voids During Electromigration

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ABSTRACT

We calculate the formation energy of small voids in Al and Cu, both at the bulk and at grain boundaries, using the Embedded Atom Method. Then, we use those results as input to a Kinetic Monte Carlo model of void nucleation and growth in Al interconnects. Preliminary test cases of the Monte Carlo model are discussed.

Keywords: electromigration; void nucleation; void growth;

INTRODUCTION

One of the major problems in microelectronic devices is the failure of metallic interconnect lines due to void formation within the line. Void formation occurs due to a combination of stress and electromigration (enhanced diffusion of vacancies due to current flow). It is currently difficult to predict the lifetime of interconnect lines, because it depends on a complex set of factors including interconnect and substrate material, interconnect microstructures, passivation method, temperature and current history, and geometry.

One of the critical questions which we investigate in this paper is the energetics of small voids in Al and Cu, both in the bulk and especially at grain boundaries. These energies are important because they control the rate at which vacancies are emitted from voids, and thus are critical in determining whether or not voids form.

Another issue which we address in this paper is studying the early stages of nucleation and growth of voids. Due to their small size, it is difficult to determine how and where voids nucleate, and it appears to be different in Al and Cu films. In this paper we present an atomic-scale model of void nucleation and growth, and discuss some preliminary tests of the model.

BULK VOID FORMATION

We begin with the study of the formation energy of voids in bulk Al and Cu, as those will serve as a good comparison to our studies of voids at grain boundaries. These calculations are similar in spirit to our earlier work [1] on the formation energies of voids in bulk Ni. The calculations in this paper were carried out using the Embedded Atom Method (EAM) [2], using well-tested potentials for Cu [3] and Al [4]. These potentials were fit to the vacancy formation energy, and also yield reasonable (but slightly low) surface energies. This is very relevant to the study of voids, which can be viewed as either a cluster of vacancies, or as an internal free surface.

The calculations were carried out using a cubic periodic cell of 4000 atoms at constant pressure. Convergence tests reveal that this size is large enough to yield void formation energies that are accurate to within 0.01 eV/atom, which is below the inherent error in the EAM potentials.

The search for the optimal void structure was not simple. We initially used our previous algorithm [1], in which the lowest energy void of n atoms was found by removing the highest energy atom from a void of n-1 atoms, and then relaxing the structure. This was satisfactory for Cu, but the Al voids required a more complete search. For voids smaller than 10 atoms, we performed an exhaustive search wherein we removed, one at a time, each possible atom next to the void and then relaxed the structure. For voids of larger than 10 atoms, we simply rescaled the Cu void structures, as they appeared to within 20 meV/vacancy of the global minimum.

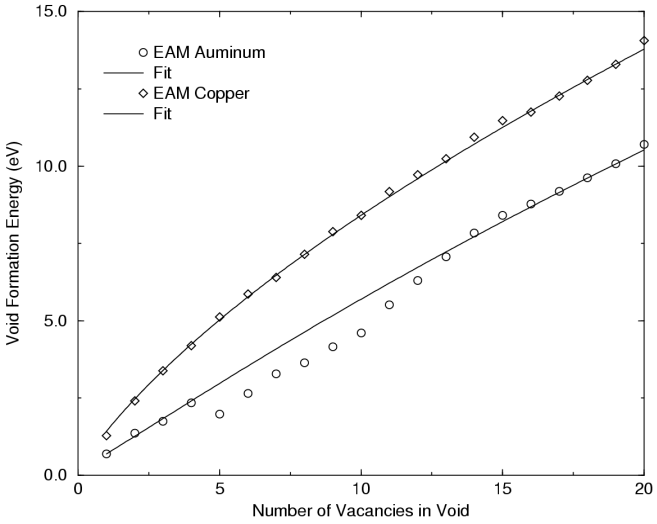

Figure 1: Void formation energies in bulk Cu and Al, as calculated with the EAM.

The results of the bulk void calculations are shown in figure 1. Figure 1 also includes a theoretical fit to the data using an expression for void energy due to Si-Ahmed and Wolfer [5],

$$E_v = 4\pi R_v^2 \gamma [1 - a/(b+N)] \quad (1)$$

where N is the number of vacancies in the void. Thus, the void formation energy is simply the surface energy of a sphere, modified by a correction factor at small sizes due to curvature effects. For Cu, we used a = 0.8 and b = 2, following Ahmed and Wolfer [5], and by fitting to a void of 19 vacancies (a closed shell), we find γ = 1240 ergs/cm^2, which is a typical surface energy. For Al, we achieved a better fit by using a = 5.92 and b = 8.6, and requiring γ to equal a typical surface energy, 925 ergs/cm^2. Overall, these empirical fits using a simple surface energy model give a good description of void formation energies. Also, it should be noted that the void formation energies in Cu are substantially higher than in Al, since Cu has both a higher vacancy formation energy and a higher surface energy.

VOID FORMATION ENERGIES IN GRAIN BOUNDARIES

To determine the formation energies of voids at grain boundaries, we used an approach similar to that above. First, we created a set of equilibrium grain boundaries by shifting one grain relative to another and relaxing, and then choosing the lowest energy configuration. This typically involved investigating 1000-2000 relative shifts of the grains, to search all likely configurations. All of the boundaries we investigated were low Σ symmetrical tilt boundaries, which were chosen to sample a full range of grain boundary energies. Thus, although we cannot study every possible boundary, we believe these are a representative sample of typical boundaries.

Next, we searched for the lowest energy void configurations at the boundaries. We began by searching all possible sites for a single vacancy, and then used that structure to, in turn, remove every possible nearby atom, to find the next largest vacancy cluster. Repeating this process for voids of up to 20 vacancies required investigating approximately 2000 void structures per grain boundary.

Void formation energies for the optimal void structures for the 6 boundaries in Al are shown in figure 2. Similar results are found for Cu, but are not included due to lack of space. One of the major results is that the formation energies of vacancies is substantially lower than in figure 1 for some of the grain boundaries. The decrease in the formation energy of the voids is found to closely correlate with the grain boundary energy. This correlation makes sense when one realizes that forming a void at a grain boundary removes part of the grain boundary, and the higher the energy of the boundary then the lower the energy of the void. Thus, a simple way to estimate the formation energy of a void at a boundary is:

$$E_v^f(N) = S\gamma - A\gamma_{gb}, \quad (2)$$

Where S is the surface area of the void, γ is the average surface energy, A is the area of the grain boundary removed, and γ_{gb} is the grain boundary energy. This equation is found to be qualitatively consistent with our results, but a richer model is needed for quantitative accuracy, due to the unusual structure of the voids as discussed below.

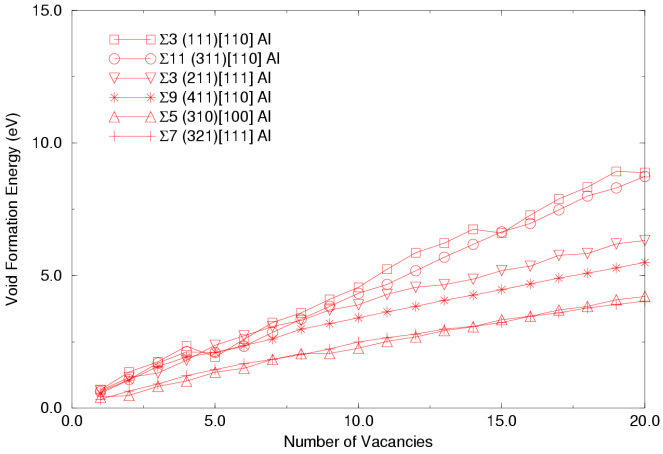

Figure 2: Void formation energies at grain boundaries in Al, as calculated by the EAM and as fit by Eq. 3.

Close inspection of the structure of the voids reveals that they are not hollow voids, but rather loose collection of vacancies, with many atoms existing between the vacancies. This is apparently due to the fact that the sites at the grain boundaries are inequivalent, and some atoms are much more strongly bonded to the network than others. Thus, the voids are really ellipsoidal regions in which some of the atoms (those sitting on weakly-bonded sites) are removed, creating a region of lower atomic density. This surprising result persists for clusters of up to 20 vacancies, and we estimate that voids of hundreds of vacancies or larger would be likely to exist as these loose clusters, rather than as a hollow void. Thus, we need to modify Eq. 2 to account for the fact that we are not completely forming a free surface, and not completely removing the grain boundary. This can be done by multiplying Eq. 2 by the correction term used in Eq. 1, yielding:

$$E_v^f(N) = (S\gamma - A\gamma_{gb})[1 - a/(b+N)] \quad (3)$$

By varying the parameters a and b, one can achieve generally good agreement with the EAM data. The agreement is slightly improved by taking into account the approximately ellipsoidal, rather than spherical, structure of the voids [6]. The results of this model are a key input parameter to the model of void nucleation and growth, discussed below.

ATOMIC-SCALE MODEL OF VOID NUCLEATION AND GROWTH

We have developed a preliminary kinetic Monte Carlo model of void nucleation and growth that explicitly includes the motion of individual vacancies through a polycrystalline Al film. In the model, we begin with a 2D polycrystalline grain structure (see Fig. 3), which is extruded into the 3rd dimension to mimic a columnar microstructure. Each grain is assigned an individual diffusion rate, based on an Arrhenius expression, with an activation energy of 0.35-0.55, chosen randomly from a truncated Gaussian distribution. Each grain is also assigned an individual grain boundary energy, chosen from the left side of a truncated Gaussian distribution. There is likely some correlation between grain boundary energy and diffusion, but the correlation has not yet been determined. The important point is that this variation in diffusion rates means that substantial vacancy flux divergences can occur, and the variation in boundary energies means that voids will form more easily on some boundaries than on others. Grain boundary junctions are treated similarly, with their properties being given by a weighted average of the boundaries that form them.

Figure 3: Typical model of a polycrystalline interconnect line.

Once these grain structures are created, the simulation begins with the random distribution of an equilibrium vacancy concentration, including in the bulk, at each grain boundary, and at each junction. Then, vacancy diffusion is allowed to occur, including motion in the bulk (with an activation energy of 0.62 eV) and along the grain boundaries and junctions. In the absence of an electrical current, vacancy motion is random, but the effect of the current is to alter the activation energy in the direction of the current, by an amount proportional to the current.

As vacancies diffuse along, they may encounter another vacancy (thus nucleating a vacancy cluster) or be captured by a void. Vacancies at grain boundaries have a chance to escape into the bulk, at a rate determined by their bulk migration energy plus the difference in formation energy. Vacancies at grain boundaries may also encounter a junction, and be captured by it. Vacancies at junctions have a chance to jump onto an adjacent grain boundary.

In addition, dislocations are assumed to serve as a source and sink for vacancies. Unlike grain boundaries and junctions, which are modelled individually, we assume the dislocations are uniformly spread throughout the bulk, so that any vacancy has the same probability of being captured, and vacancies are emitted throughout the bulk at a rate that would maintain the correct equilibrium vacancy concentration, in the absence of external effects (like current). Later versions of our code will include the effect of dislocation capture at grain boundaries and junctions.

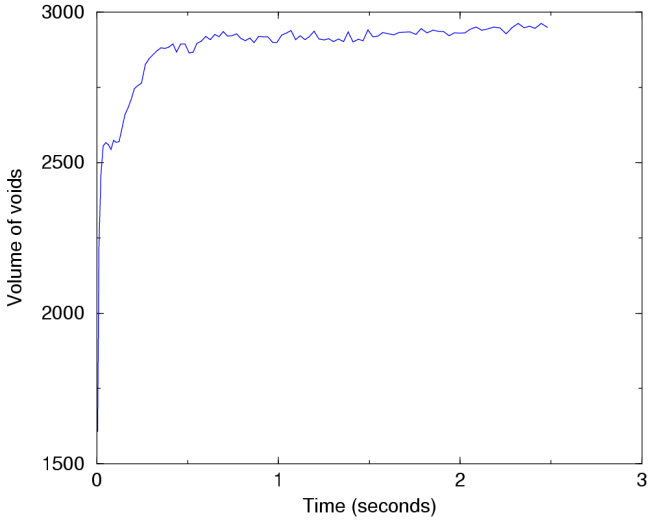

Figure 4: Number of vacancies in voids as a function of simulation time.

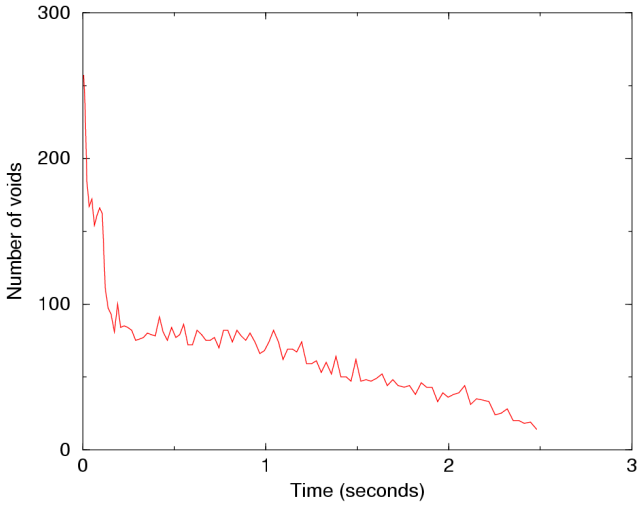

Figure 5: Number of voids as a function of simulation time; combined with Figure 4, this is a classic indication of Ostwald ripening.

All of the rates described above are incorporated into a master rate table, and events are chosen according to a weighting proportional to their relative weight. Thus, at each MC step, an event is randomly selected and executed.

We have tested this preliminary version of our model on the line shown in Figure 3 for several sets of conditions. The line is 5 microns by 1 micron by 100 Angstroms (this thickness is sufficient to allow simulation of void

nucleation in a typical portion of a film). Each trial involves 2 x 10 9 MC steps. In the last half micron of the line, the current is assumed to go linearly to zero, mimicing the behavior at the end of a line. For the test cases, we assume there is no flux into the line, for easier evaluation of the code, but later versions of the code will include this flux properly. For test cases of thermal equilibrium vacancy concentration and no current bias, vacancies move properly and occasionally form di- and tri-vacancies, but do not form stable voids.

At elevated concentrations (100 x thermal equilibrium at 323 K), for an artifically high bias (0.02 eV), we do observe rapid diffusion of vacancies towards the end of the line. Over 200 voids form, mostly at the end of the line, with a few occurring earlier in the line. As shown in figures 4 and 5, the number of vacancies in voids quickly stabilizes, but the number of voids decreases as time progresses. This is a classic example of Ostwald ripening, with some voids reaching the size of several hundred vacancies.

These simple test cases demonstrate that the code appears to be working properly, with voids not forming when they should not, and forming when they should. Future work will include several changes to the code, including much lower biases (typical biases are in the range of 10^{-5} eV), capture and emission of vacancies by dislocations intersecting grain boundaries, flux into the lines, and the effect of stress on vacancy motion and void evolution.

CONCLUSION

We have calculated the formation energies of Al and Cu voids in the bulk and at grain boundaries, and have explained those results in terms of a simple, physically-based model. We have incorporated those results in a preliminary atomic-scale model of void nucleation and growth, and future extensions of the model were discussed.

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REFERENCES

[1] J.B. Adams and W.G. Wolfer, J. Nucl. Mater. 166 (1989) 235.

[2] M.S. Daw and M.I Baskes, Phys. Rev. Lett. 50 (1983) 1285.

[3] S.M. Foiles, M.I. Baskes, and M.S. Daw, Phys. Rev. B 33 (1986) 7983.

[4] F. Ercolessi and J.B. Adams, Europhys. Lett. 26 (1994) 583.

[5] Si-Ahmed and W.G. Wolfer, in Effects of Radiation on Materials: Proceedings of the 11th Annual Symposium, Vol. 782 of ASTM STP, edited by H.R. Brager and J.S. Perrin (American Society for Testing and Materials, Philadelphia, PA), pp. 1008-1022.

[6] David F. Richards, PhD thesis, University of Illinois (1999).