MICROSCOPIC ESTIMATES FOR ELECTROMIGRATION VELOCITIES OF INTRAGRAINULAR Voids IN THIN ALUMINUM LINES

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ABSTRACT

We explore the effect of faceting on possible mechanisms for mass transport around electromigration voids in aluminum interconnects. Motivated by linear response estimates which suggest that particle flux would be much higher along steps than across terraces on a clean aluminum surface, we study step nucleation in the presence of a small driving force along a surface. We find that step nucleation, even on a nearly defect-free void surface, would be slow if the step energy is equal to that calculated for a clean aluminum surface. In the presence of a uniform electromigration force, the creation of new steps between existing ones should not occur unless the free energy cost of a step is much less than thermal energies. We conclude that voids cannot move intragranularly at $\mu$m/hr rates without help from other factors such as local heating and impurities.

INTRODUCTION

The increasing miniaturization of aluminum interconnects in VLSI circuits has produced an urgent need for new insight into electromigration phenomena. Although researchers have arrived at useful models for particle motion along grain boundaries in wide aluminum lines, lines with micron width or smaller tend to have a “bamboo” structure which lacks continuous grain boundary paths, and different electromigration mechanisms can dominate in these small lines. Electromigration voids move through single grains, typically along the edge of a line [1]. Failure often occurs in the middle of a grain, where voids can collide to make a large hole or one void can collapse into a transverse slit [2] [3]. Electron microscope observations suggest that collapse tends to occur after a void moves into a grain with the appropriate orientation [4]. Thus, it seems that void motion is crucial to both of these forms of failure. But what microscopic processes are actually happening as those voids move?

One great help in modeling this flow is the weakness of the electromigration driving force. The force $F$ induced by a current density $j$ and resistivity $\rho$ follows the linear relationship $F = Z^* e \rho j$, where observations of macroscopic behavior give the proportionality constant in aluminum as high as $Z^* \sim 20$ [6]. For typical testing conditions in aluminum interconnects, with current density $> 10^6$A/cm$^2$ and temperature 500-600K, this driving force has to move an atom through roughly an entire micron before it does $1kT$ of work. Although current concentration near voids, resistivity variation at the void surface, and orientation of the void surface will modify the size of the electromigration force, the bulk value provides a useful starting estimate for surface calculations, and it certainly indicates that the driving force is a small perturbation to surface diffusion.

For simplicity, previous models of flow around the edge of a void have often assumed a cylindrical void, where all atoms on the surface participate in diffusion with an estimated average mobility [7]. In contrast, observed voids in thin interconnects usually show clear facets, particularly on their leading face. Examination shows such facets to have (111)
Since the energy required to dislodge an atom in an Al(111) terrace is very high, flow across void a surface should probably be modeled by first asking how many adatoms (or vacancies) are available for surface diffusion, and then, if this number is very low, checking to see if motion along steps should dominate the mass flux. The latter will depend, in part, on step density at the void surface, and we will explore this issue at some length.

**Linear Response on Al(111)**

To calculate the lowest order term in this flux, we assume that the density of the mobile species is unchanged when the force is turned on and simply moves according to linear response:

\[
\text{flux} = \frac{D}{F/kT} n(x) - D \frac{dn}{dx},
\]

where \(D\) is the diffusion constant and \(n(x)\) is the local density of mobile diffusers. Near a straight step, the equilibrium density of adatoms at a certain type of site is given by the free energy cost of moving an atom from a kink site on the step to the type of spot in question, which might be on the surface or resting against the step \([9]\). Thus, we model the first term above as a simple function of force, temperature, and diffusion barriers. Recent density functional calculations carried out in the local density approximation (LDA) by Stumpf and Scheffler \([10]\) allow an estimate of this lowest order flux term for adatoms on both a clean Al(111) surface and at steps on that surface parallel to the driving force \([11]\). To do so, we assume a typical diffusion attempt rate of \(10^{12}\) Hz and obtain flux estimates from (1) in units of atoms/s along an atom column. (The actual attempt rate for the exchange process in \(\{111\}\) step diffusion may be an order of magnitude higher \([10]\).)

| structure  | adatom cost | ad. density | diffusion barrier | hop time | atoms/s/column |
|------------|-------------|-------------|-------------------|----------|----------------|
| (111) surface | 1.05 eV     | \(8 \cdot 10^{-10}\) eV | .04 eV          | \(2 \cdot 10^{-12}\) s | .1             |
| \{111\} step | .28 eV      | \(4 \cdot 10^{-3}\) eV | .42 eV          | \(4 \cdot 10^{-9}\) s | 300            |
| \{100\} step | .25 eV      | \(7 \cdot 10^{-3}\) eV | .32 eV          | \(6 \cdot 10^{-10}\) s | 3500           |

*Table I. Estimates at 580K and current density \(\approx 5 \cdot 10^6\) A/cm², using density functional results by Stumpf and Scheffler.*

Under testing conditions, observed void velocities seem to range from a micron every few hours to over 1 \(\mu\) m/hr (although some voids are stationary). A micron sized void with velocity 1 \(\mu\) m/hr would have to move roughly \(4 \cdot 10^3\) atoms/s through each atom column on its surface. The estimates above would only approach this flux for a dense network of steps. The estimates in Table I are not, of course, a quantitative prediction for adatom flow in real electromigration voids. Stumpf and Scheffler find that energy differences in their calculations are converged to within .06 eV, but use of the local density approximation at a surface may introduce some additional error. More importantly, voids do not have clean aluminum surfaces, and we will discuss this issue below. Still, this estimate of particle flux on clean aluminum steps and terraces yields two conclusions. First, unless void surfaces are covered with steps, **something** must be raising particle flux there far above the rates expected for clean Al (111). Second, unless contaminants change the ratio of step to surface flow by orders of magnitude, steps on a dirty aluminum surface will remain competitive routes for mass flow. Both conclusions raise the issue — what step density should be expected on void surfaces?
STEP NUCLEATION MODELS

As a void moves, its leading side continually uncovers new sections of (111) surface. Thus, if the leading surface of the void contains a high step density, new steps must constantly nucleate there \cite{13}. Since this surface of the void is losing mass, new steps will tend to appear through pits in the surface which arise from fluctuations and will grow if they become larger than a critical size. An external driving force can affect step density by changing this critical pit size, but we will find that the weak force present during electromigration cannot produce rapid step production.

First, we consider the most favorable case in which a driving force could enhance step nucleation. If a pit appears where there is no incoming flux of adatoms, the pit will reach critical size when it attains equilibrium with its downstream environment, taken to be a straight step that is a distance $L$ from the pit. This equilibrium must balance two effects: when the driving force $F$ moves an atom from pit to step it gives the atom an energy $-F \cdot L$, but taking an atom out of the pit increases its size and increases the energy cost of its perimeter by an amount $g/R$, where $g$ is a step free energy per unit length, and $R$ is the radius of the pit. Thus, when this radius is larger than $g/(F \cdot L)$, the pit will tend to lose more and more atoms to the downstream step; tiny pits will disappear and not contribute any new steps to the system.

Even this most favorable configuration for step nucleation produces a rather high estimate for critical pit size on an electromigrating surface. Recall that the electromigration force does an amount of work of order 1 kT (i.e. of order .05 eV) in moving an atom through a micron — a void size! Stumpf and Scheffler find that step energies on the Al (111) surface are between .23 and .25 eV/ lattice site \cite{12}. Thus, even our extreme model configuration with $L$ as large as a micron would lead to a critical pit radius between 4.5 and 5 lattice sites. The corresponding critical pit energy, $g (2\pi R_c) - \pi R_c^2 F L$, is between 3 and 4 eV for these estimates and provides a substantial barrier to nucleation.

In a more realistic case, the pit which appears through thermal fluctuations will lie between two steps. A stable pit must be in equilibrium with the adatom density around it, in the mass flow between the upstream and the downstream step. To find the adatom density required for pit equilibrium, we turn to a surface with no driving force. There, Gibbs–Thomson theory predicts that mass will flow into a pit unless the adatom density around it is suppressed relative to the equilibrium density near a straight pit by the factor $e^{-g/(RkT)}$ \cite{15}, where $g$ and $R$ were defined above. If a driving force is present, can it kinetically suppress the adatom density between two steps by a factor equal to the Gibbs–Thomson suppression near an equilibrium pit?

![Figure 1 Toy model of energy landscape for adatom diffusion between steps.](image-url)
To answer this question, we consider a toy model for a parallel step array, whose energy landscape for adatom diffusion is shown in figure 1 [14]. The adatom density profile between the steps must be a solution of the driven diffusion equation \( D d^2 n/dx^2 - D kT \frac{F}{kT} dn/dx = 0 \). Boundary conditions must match the flux in the central region between steps with the rate at which particles enter and leave the supply of adatoms attached to each step. For small flux between steps and relatively slow diffusion along a step, the density of step adatoms should be very close to the equilibrium value [14]. Imposing this step density as a boundary condition for the energy landscape with constant barriers (ES=0 in figure 1), yields an adatom density between the steps which is constant and equal to its equilibrium value. In this case, the driving force is unable to produce the suppression of adatom density required for a pit to be in equilibrium. Without an extra Ehrlich-Schwoebel barrier for motion at a step, a uniform electromigration force should be unable to induce any pit nucleation between steps.

If there is an extra barrier for leaving a step (designated ES in figure 1), then the adatom density will vary between steps. Figure 2 shows this variation across a step separation of 100 lattice sites, for \( ES = 2kT \) (a value motivated by the LDA results) and two different force strengths. These density results are relatively insensitive to step separation. If a pit appeared between two long parallel steps with these barriers, then far away from the pit the adatom density would follow the solution from the toy model. Mass would flow towards the pit from the far region unless the local adatom density near the pit was as large as the corresponding toy model result. Thus, a critical pit near the upstream step would have a radius such that \( e^{-g/R_c kT} \) was equal to the kinetic suppression of adatom density near the upstream step in the toy model result. The results in figure 2 for \( Fa = .001 \) (a large force for an electromigration problem) show a kinetic suppression of .994, which corresponds to a huge critical pit size unless \( g/kT < 1 \). Thus, even when there is an extra Ehrlich-Schwoebel barrier at steps, the weak driving force expected in electromigration should be quite ineffective at inducing pit nucleation.

Figure 2. Adatom density between steps as fraction of equilibrium value for \( ES = 2kT \) and two values of the driving force. Note that the smaller force value here is larger than that in many electromigration tests and yet corresponds to a minimal kinetic suppression of the adatom density. (Note: \( a \) is a lattice spacing.)
OTHER INFLUENCES

So, if an electromigration void contained ideal Al (111) surfaces, then the leading face of the void would contain very few steps and the flow across that surface would be far too low to allow the void to move at a $\mu$m/hr rate at testing temperatures. Yet, voids do move. What additional factors are important in real voids? First, some evidence exists for intense local heating near voids at large current densities. Where such thermal spikes were measured, current density throughout the wire was an astounding 48 MA/cm$^2$ \[17\]. Other observations suggested that local melting can occur near voids which nearly breach an interconnect \[2\]. There, the macroscopic current density of 5MA/cm$^2$ would have been magnified by current concentration. At such huge current densities, impediments to heat flow, such as local loss of thermal contact with the base, might produce the dramatic heating observed. Since such heating effects go as $J^2$, they should be far less important at normal testing currents with less constriction. Novel heating mechanisms may also be important near $10^8$A/cm$^2$. \[18\]

In addition, real void surfaces are not clean. Many interconnects are doped with copper, which is known to produce a small enhancement of bulk aluminum diffusion \[19\]. If residual etchant from the lithography process contaminates large regions of the void surface, it could dramatically change aluminum flow and surface structure. And, of course, exposed void surfaces will oxidize. Recent observations of interface mass loss suggest that mobility at a boundary between aluminum and a full aluminum oxide layer can be high — perhaps approaching that along the fast diffusion paths at aluminum grain boundaries \[21\]. Still, this phenomena may not be ubiquitous, since STM observations found that oxidation of the first layer or so of an Al(111) surface suppressed step diffusion and appeared to freeze the surface topography in place \[23\].

Even if a specific impurity is found to be key for rapid void velocity, a determination of the mechanism for enhancement will still be of interest. If contaminants can eliminate most of the free energy cost of step production on the close-packed Al (111) surface, then the leading surfaces of electromigration voids may be covered with enough steps to explain observed transport. If not, these surfaces should be highly faceted and enhanced flow must occur between steps. To move 4000 atoms/s through every column on a surface at quoted testing temperatures, linear response estimates require the sum of adatom (or vacancy) production cost and corresponding diffusion barrier to be about half that given for adatoms on clean aluminum terraces. Perhaps further study will pinpoint a contaminant that can produce such dramatic changes throughout a void surface.

CONCLUSIONS

Linear response estimates of mass flux on a clean Al(111) surface are far too low to explain observed void motion at standard testing conditions unless void surfaces are covered with a dense network of steps. As layers of atoms are removed from the leading surface of a void, the electromigration force should be too weak to induce substantial nucleation of new steps unless the step free energy is nearly zero. Although heating effects seem to enhance void velocity at extremely high current density, impurities may play a vital part in boosting void velocity at standard testing conditions. Two different mechanisms for mobility enhancement could occur — reduction in step energy or an increase of mass flow between steps. Since these various mechanisms can scale quite differently with current density and temperature, understanding the sources of high void mobility during laboratory electromigration tests should help in determining whether related mechanisms are important to failure under normal interconnect operation.
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