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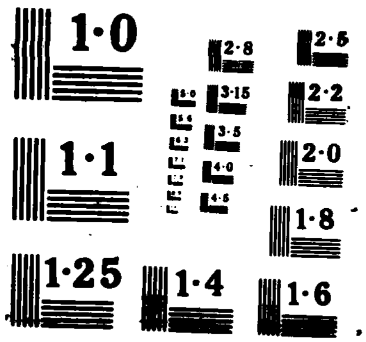
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COMPUTER SIMULATION OF DETERIORATION BY ELECTROMIGRATION

Rensselaer Polytechnic Institute

H. B. Huntington and S. Ahmad

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Analysis of electromigration and redistribution of material in grain boundaries has been programmed for simulation of these processes in relatively realistic grain boundary networks generated from computer generated Voronoi networks. Realism is improved by simulation of annealing prior to simulation of electromigration.

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Evaluation

This work has provided some much needed analysis of the conditions of electromigration in models of greater realism than have heretofore been attacked. The progress has been good considering the complexity and ambitiousness of the task. Further effort would be well advised.

MARK W. LEVI
Project Engineer

I. Planning and Survey Stage

The work began with a computer search for relevant material published during the last two years in the Chemical Abstracts and Physics Abstracts. From the Chemical Abstracts a total of 113 references responded to a call from the key words "electromigration" and "electrotransport". These were surveyed for applicability and availability and 26 rated high on both counts. The corresponding reference list was much longer for the Physics Abstracts. It was decided to require also mention of "thin film" as a key phrase and this reduced the list substantially - to 25. All seemed pertinent and were provided with substantial abstracts. There was naturally a considerable degree of overlap between the two lists. This background has proved most useful in selecting a topic for in depth study and also in giving a general picture of the most recent aspect of electromigration problems.

II. Generation of Grain Boundary Network.

In the course of this literature survey there surfaced one particularly pertinent paper by K. Nikawa[1], which described a detailed computer simulation, using Monte Carlo methods, of a rather simplified model of stripe deterioration by grain boundary transport. The accompanying reference list [2-5] includes several earlier papers in the general field. It was in this area we decided to concentrate our computing efforts.

The first step in this procedure was to devise a system for generating a realistic grain boundary network. This was planned as a two step process.

A. First a random network of grains was generated according to the Voronoi prescription, which has been discussed in a review article by Weaire and Rivier[6]. The method is to establish a random placing of points in two dimensions. Next one constructs the perpendicular bisectors between all pairs of adjacent points and portions of these lines now constitute the grain boundaries of the network. The physical interpretation could be that the random points correspond to nucleation centers for crystallization which grow uniformly until they meet at the perpendicular bisectors, i.e. grain boundaries. In programming this concept for a stripe of a particular width we made use of a prior program[7] by I. K. Crain for a limited network and were successful in generating reasonable structures for different size grains. As a last step grain orientations were established by Monte Carlo selection.

B. Next an effort was made to equilibrate the intergranular tensions at the vertices of the network. We assumed that these tensions would practically equal to the intergranular energies (on the assumption of negligible temperature dependence). For these energies a dislocation model was again invoked which set the grain boundary energy proportional to the dislocation density or $\sin \frac{\theta}{2}$ for $\theta < 37^{o}$ and kept the energy constant for $\theta > 37^{o}$, where θ is the angle of misorientation between the adjacent grains. Since the grain boundary diffusivity also varies in somewhat the same way as the tension, it seemed desirable, perhaps even important, to try to establish tension equilibration. This proved, however, quite a difficult business, as might have been anticipated for a multidimensional search for a equilibrium configuration. For a time this effort was shelved in favor of an exploration of the actual mass motions with the grains.

III. Modelling the Electromigration Process

A. Characteristics of the grain boundaries

The key quantity in the simulation process is $m_{\sigma}(x,t)$, the amount of matter in grain boundary segment (denoted by subscript σ) per unit length. Initially all grain boundaries are assumed ungrooved and the m_{σ} have a constant value $m_{o} = Nd_{o}\delta$ where N is the number of atoms per unit volume, d_{o} is the thickness of the stripe film and δ is the (nominal) width of the grain boundary segment. In some regions $m_{\sigma} > m_{o}$ and there is matter build-up which continues until $m_{o} \sim m_{M}$ at which point extrusion starts. In contrast to those grain boundaries which show matter excess there are others which show matter deficit $m_{\sigma} < m_{o}$. Because these regions are critical in void formation their treatment is more detailed and complex. Matter deficit in the grain boundaries (vacancies) tends to condense as grain boundary grooves at the surface. As we show later, the number of vacancies still in the grain boundary is relatively small after a short initial period. The matter missing in the grain boundary grooves, per unit length of grain boundary, is taken to be $Nd_g^2 \tan \beta$ ($\tan \beta$ is small and has been arbitrarily set at 0.1) where d_g is the depth of the groove and β is the angle at the groove base.

With the appearance of the grooves another mechanism for mass transport becomes operative - surface motion down the groove walls. (Presumably surface diffusion over the upper surface of the stripe is inhibited by a passivating layer.) This process should proceed rapidly and be independent of the original grain misorientation at the boundary. Its effect is to widen the groove and therefore a new quantity, w(x,T), is introduced which denotes the grain boundary width at the surface for each point along the segment. This action greatly increases the effective β so that $\beta \to \beta'$ where $\tan \beta' = \frac{w}{2d_g}$

In addition to the m(x,t) quantities to describe the state of the segment, one might also consider g(x,t), the groove volume per unit length. It appears, however, that, in general, $g(x,t) \div (m_o - m(x,t)$ will be close to unity, since the vacancy volume in the grain boundary is relatively small.

B. Equations for mass motion

Within the grain boundary the appropriate mass transport equation is

$$\frac{\partial m(x,t)}{\partial t} = \frac{\partial}{\partial x} \left\{ D_{\sigma\perp} \left[\frac{\partial m(x,t)}{\partial x} - A\, m(x,t) \right] \right\} \qquad (1)$$

Distance along the grain boundary segment is denoted by x. The grain boundary diffisivity is $D_{\sigma\perp}$ where σ again numbers the segment. We show in next section $D_{\perp\sigma}(\theta)$, where θ is the misorientation angle between the grains meeting to form the boundary. The coefficient of the driving force term, A, is $A_o \cos \phi$ where ϕ is the angle between the grain boundary and direction of E and A_o is $\frac{|e|EZ^*}{kT}$ about 0.1μm for $E = 2.2$V/cm, $Z^* = 20$ and $T \sim 150°$ C. All changes in m are treated on an equal basis, whether they arise from changes of vacancy concentration in the grain boundary or a gradient in groove depth.

Preparatory to setting the equation up for computer application each segment had its length divided into a discrete number of evenly spaced check points. The spacing is denoted by a and is roughly about 0.2μm for all segments. Eq (1) is now written

$$\frac{\partial m(x,t)}{\partial t} = \frac{D_{\perp\sigma}}{a}\left[\frac{m_{n+1} - 2m_n + m_{n-1}}{a} - \frac{m_{n+1} - m_{n-1}}{2} A_\sigma\right] \qquad (1a)$$

Where the digitized values fo` ` have been used on the right. At the ends of the segments ($n = 0$ or n_t) _ equation is slightly altered.

$$\frac{\partial m(0,t)}{\partial t} = \sum_\sigma \frac{D_{\perp\sigma}}{a}\left[\frac{m_1 - m_o}{a} - A_\sigma m_1\right] \qquad (1b)$$

In a similar way the surface motion on the groove walls can be expressed in terms of g(x, t) = N x volume of the groove/length.

$$\frac{\partial g(x,t)}{\partial t} = \frac{\partial}{\partial x} D_s \left[\frac{\partial g(x,t)}{\partial x} - A_s\, g(x,t)\right] \qquad (2)$$

Where D_s is the diffusion on the free surface and A_s is the surface driving force. As before the digitized version is

$$\frac{\partial g}{\partial t} = \frac{D_s}{a}\left[\frac{g_{n+1} - 2g_n + g_{n-1}}{a} - A_s \frac{g_{n+1} - g_{n-1}}{2}\right] \qquad (2a)$$

and for the segment ends

$$\frac{\partial g_o}{\partial t} = \frac{D_s}{a}\left[\frac{g_1 - g_o}{a} - A_\sigma g_1\right] \qquad (2b)$$

(In a later section we give an argument why the diffusion term should be omitted from eq. 2.)

C. Assumed stripe structure

It is reported that most metallized stripes, particularly for aluminum, exhibit a pronounced {111} structure. Such a structure implies that pure tilt interfaces constitute most of the grain boundaries. If we invoke a dislocation model for the small angle grain boundaries, these would then consist of edge dislocations directed perpendicular to the substrate, hence the notation $D_{\perp\sigma}$ for diffusion in the stripe, perpendicular to the dislocations. Accordingly the assumption is made that for large angle grain boundaries ($\theta > 37^o$ as a nominal dividing line), diffusion is isotropic at a value D_l. Holding to the dislocation model for grain boundaries one obtains for the diffusion parallel to the dislocation and directed perpendicular to the substrate

$$D_{\parallel} = D_l \sin\theta/2/\sin 37^o/2 \qquad \text{for } \theta < 37^o \tag{3}$$

For diffusion along the stripe one modifies a formula of Li to get

$$\frac{1}{D_{\perp}} = \frac{1-\alpha_o}{D_o} + 6\,\frac{\alpha_o}{D_l} \tag{4}$$

where D_o is the diffusion through the bulk and $\alpha_o = r_o/h$. Here r_o is the dislocation core radius, $b/h = 2\sin\frac{\theta}{2}$ and b is the Burgers vector. (The original Li formula was $\frac{1}{D} = \frac{1-\alpha_o}{D_o} + \frac{\alpha_o}{(1-\alpha_o)D_o + \alpha_o D_l}$). Nominally $\alpha_o = \frac{\sin\theta/2}{\sin 37^o/2}$.

D. Difficulty with Diffusion

The direct integration of equs (1) and (2) poses a problem in that useful convergence of the diffusion part requires some sublety in method and a very considerable number of time steps. In terms of an average segment length L_{Av} the natural time constants of the system are $[D_l\ L_{Av}^{-2}]$ (about $.6 \times 10^3$s) and $[D_l\ A\ L_{Av}^{-1}]$ (about 5×10^3s). As both of these constants are very short, of the order of an hour, it is clear that the approach to void formation must not be limited to time steps of such small size. Accordingly a procedure was developed to integrate over a longer period.

E. Steps in the program simulation

The individual stages that are involved in each time step are here described in order, somewhat after procedure used in the twelfth status report.

a.) First stage - matter accumulation (or depletion) at each vertex, F_V, in accord with eq (1b),

$$F_V = \sum_{\sigma} D_{\sigma\perp} \left[\frac{(m_1 - m_o)}{a} - A_{\sigma} m_1\right],$$

where the σ-summation is over the segments which meet at the vertex in question. For the first time-step all the m's are equal and only the A_σ term contributes.

b.) Redistributing F_V among the segments meeting at V.

For each segment a portion of F, namely f_σ, is redistributed as a flux coming into the segment.

$$f_\sigma = F_V D_{\sigma\perp}^{\frac{1}{2}} / \sum_{\sigma} D_{\perp\sigma}^{\frac{1}{2}} \qquad (5)$$

c.) Method of redistribution

The thin film solution for the diffusion equation is used, working from both ends of the segment,

$$a \frac{\partial m(x,t)}{\partial t} = f_\sigma \frac{1}{(\pi D_{\perp\sigma} t)^{\frac{1}{2}}} e^{-x^2/4D_{\perp\sigma} t} \qquad (6)$$

One would like to be able to state what m(x,t) is at time t.

Integration gives $m(x,t_1) = (\pi)^{\frac{1}{2}} f_\sigma D_\sigma^{-1} x \, \zeta\left(\frac{x}{2(D_\sigma t_1)^{\frac{1}{2}}}\right)$ where $\zeta(y) = \frac{e^{-y^2}}{y} - \sqrt{\pi}\,\mathrm{erfc}\, y$.

This integration technique allows one to greatly increase the time, from 10^4 to 10^6 seconds. For such long times, however, the diffusion thin-film solution will usually have a large value at the opposite end of the segment. These "tails" have to be evaluated by integrating m(x) from x_1 to ∞,

$$\int_{x_1}^{\infty} m(x)\, dx = \frac{2f}{\pi^{\frac{1}{2}}} t_1 \eta(y_1) = T(x_1,t_1) \qquad (7)$$

where $\eta(y_1) = (1 + 2y_1^2) \int_{y_1}^{\infty} e^{-y^2} dy - y_1 e^{-y_1^2}$ and $y_1 = \frac{x_1}{2\sqrt{D_{\sigma\perp} t_1}}$. One then sums the $T(L_\sigma,t)$ at each vertex for the "tail" contribution from all the segments that meet there. This gives a new F_2 which is then iterated to give smaller contributions to the $m_\sigma(x,t_1)$ of the network.

d.) After these "tailing" corrections have converged, the next stage is to consider the grooving that occurs near those vertices where a material deficit has developed. If $m(x,t_1) - m_o < 0$, it is reasonable to expect large fraction of this deficit will be converted into the grain boundary groove volume, $g(x, t_1)$, or

$$g(x,t_1) = K(x,t_1)\,\{m_o - m(x,t_1)\} = K(x,t_1)\, m_1(x,t_1) \tag{8}$$

$K(x,t_1)$ can be estimated from a model wherein the diffusion of vacancies in the z-direction (upward from the substrate) is explored. Suppose $m(x,z,t_1) = m(x,t_1)\, Z(z)$ where

$$Z(z) = \frac{\pi}{2d_b} \cos \frac{\pi z}{2d_b} \tag{9}$$

Here $z = 0$ at the substrate and $z = d_b$ at the bottom of the groove, $d_b = d_o - d_g$ where d_g is the groove depth. Introduce now $T(x,t_1)$, the number of vacancies still in the grain boundary, $T(x,t_1) = m_1(x,t_1) - g(x,t_1)$

$$\frac{\partial\, T(x,t)}{\partial t} = -\lambda_\sigma T(x,t) + \frac{\partial m_1(x,t)}{\partial t}\,. \tag{10}$$

Here $\lambda = D_\parallel(\theta) \left(\frac{\pi}{2d_b}\right)$ from the equation for diffusion perpendicular to the substrate and $\frac{\partial m_1}{\partial t}$ could be taken from (eq 6) - if tailing correction is neglected.

To get a rough solution disregard the Gaussian factor since long times are involved. Roughly then $\frac{\partial m1}{\partial t} \sim A\, t^{-\frac{1}{2}}$ and $m \sim 2A(t_1^{\frac{1}{2}} - t_m^{\frac{1}{2}})$ when t_m is a short time cut-off which replaces the exponential.

$$\frac{\partial T}{\partial t} = -\lambda T + A\, e^{\frac{1}{2}} \tag{10a}$$

Discarding the homogeneous solution $ce^{-\lambda t}$ we have for T

$$T(t) = Ae^{-\lambda t_1} \int_{t_n}^{t_1} e^{t'\lambda} (t_1 - t')^{-\frac{1}{2}} \, dt' = A \int_o^{t_1} e^{-\lambda\tau} \tau^{-\frac{1}{2}} \, d\tau$$

$$T(t) = 2A\, x^{-\frac{1}{2}} [\varepsilon rf(\lambda^{\frac{1}{2}} t_1) - erf(\lambda^{\frac{1}{2}} t_m)] \sim 2A\, \lambda^{-\frac{1}{2}}$$

and finally $K(x,t) \simeq \{1 - (\lambda t_1)^{-1}\}$ (11)

Often K(t) is close enough to unity to neglect the difference. Actually the form of (9) is quite independent of the formula for $\frac{\partial m_1}{\partial t}$. To determine d_g the groove depth we assume it to be V-shaped with a small vertex angle β. Then

$$g(x) = N\, d_b^2 \tan \beta \tag{12}$$

e.) The treatment of the surface diffusion along the walls of grooves bears a close resemblance to the procedure of the earlier sections dealing with diffusion in the grain boundaries. We use the results of section D for d_g to determine F_{sv}, the quantity analogous to F_v of section (a)

$$F_{sv} = -\frac{\Sigma}{\sigma} D_s A_{s\sigma} 2d_{g\sigma v} \sec \beta. \tag{13}$$

Here D_s is the surface diffusivity which characterizes the free surface. (Our model presumes that, without grooving, there is no free surface because of oxydizing or passivating films.) The $A_{s\sigma}$ is the driving force coefficient for the surface and equals $A_s \cos \phi_\sigma$. The $d_{g\sigma V}$ is the groove depth for the σ segment at the V vertex. The diffusion contributions to (11) have been omitted since the surfaces of the groove walls are smooth and there is no preferred direction for matter diffusion. It is implied that there is no electromigration-driven pile-up of vacancies along the groove wall surfaces.

As before the F_{sV} is divided into $f_{s\sigma}$, which are now all equal since D_s is independent of σ. The back distribution into the segments now gives rise to two different possibilites: segments that show deficits at both ends and those which show deficit at one end only. Without the pure diffusion term the mass motion equation becomes

$$\frac{\partial G_\sigma(x,t)}{\partial t} = -D_s A_{s\sigma} \frac{\partial G_\sigma(x,t)}{\partial x} \tag{2c}$$

The quantity $G(X,t)$ is that groove volume, over and above $g(x,t)$ previously defined, which is acquired by virtue of the surface mass motion.
A useful long time solution for this equation is

$$G_g(x,t) = B_1 - B_2 x + B_2 D_s A_s t \tag{14}$$

where B_1 and B_2 coefficients are fitted to flux conditions at the vertices or zero flux condition for those grooves that terminate in a segment (single-ended grooves). If we hold to the V-shaped groove model then $G = d_g \tan \beta'$ where now $\beta' \gg \beta$ and β' may be a large angle. The details of the solution of this surface aspect have not yet been completely worked out.

f.) The regions of material excess require less detail than those showing deficit. We expect to select a criterion for the breaking of the passivating layer by internal pressure. After this is exceeded the local mass build-ups with time will cease as the extra material is extruded.

F. Present situation and future directions.

Programming has proceeded to the point of stage c, as detailed in section E. Trial runs on a single grain have proved satisfactory. Further work should incorporate the remaining stages and enlarge the operating field to a full stripe. As one proceeds with ensuing time steps the grooves become incised deeper and surface diffusion replaces grain boundary diffusion as the principal mode of mass transport. For the cases where voids have developed a somewhat different program of operations will be needed. It is quite problematical how to bring consideration of electrical and thermal effects into play but they certainly should be considered.

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