Electromigration drift velocity in Cu interconnects modeled with the level set method

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Electromigration (EM) drift velocity (DV) experiments in polycrystalline pure Cu lines are simulated numerically with the level set method. The simulation is based on a grain boundary (GB) grooving model, incorporating an electric field. The model is distinguished by two key requirements imposed at the triple point where two surfaces and a GB meet: that of GB and surface flux coupling (flux continuity), and that of permanent equilibrium between surface and GB tensions. Surface diffusion exists only at the advancing cathode edge, and is driven both by local curvature gradients and by the local field. Using independent, literature diffusivity values, the simulation yields both the DV prefactor and the EM activation energy in an Arrhenius-type expression. An excellent match is obtained with experimental DV values in the T range of 573–723 K. Some implications regarding the material transport mechanism are discussed. © *2000 American Institute of Physics.* [S0003-6951(00)01647-8]

Drift velocity (DV) experiments, first introduced by Blech and Kinsborn,[1] are generally accepted as providing the most physically transparent illustration of electromigration (EM). As shown schematically in Fig. 1, the average EM velocity V_{EM} in the line is given by the displacement L of the cathode edge (''front'') divided by the drift time. If the front advances uniformly, L (and V_{EM}) can be measured relative to any location on the edge. V_{EM} follows an Arrhenius type dependence on temperature T:

$$V_{\mathrm{EM}}=(V_0)_{\mathrm{EM}}\exp(-E_{\mathrm{EM}}/kT), \tag{1}$$

where $(V_0)_{\mathrm{EM}}$ is the pre-exponent factor and E_{EM} is the EM activation energy. The literature data providing both $(V_0)_{\mathrm{EM}}$ and E_{EM} remain surprisingly sparse. For copper interconnects, most of it has been listed in Ref. 11, with additional reliable data provided by Hu *et al.*[2]

We have recently introduced a two-dimensional numerical simulation of EM in polycrystalline lines[3,4] based on the level set method.[5] The numerical algorithm is formulated along the lines of a previous analytical grain boundary (GB) grooving model,[6] and incorporates in addition an electrical field. One key element in both models is that of ''coupling'' between GB and surface material fluxes (J_{GB} and J_s, respectively) assuring flux continuity at the triple point where two grain surfaces meet their common GB, see Fig. 1. This condition reads as $J_{\mathrm{GB}}=2J_s$. While self-evident in its importance as a physical explanation of how material is transported along the line, this element is missing in most models dealing with EM drift. Another condition is that of permanent equilibrium between GB and surface tensions at the triple point (groove root), i.e., $\gamma_{\mathrm{GB}}=2\gamma_s\sin\theta_0$, where θ_0 is related to an equilibrium dihedral angle φ by $\varphi=2(\pi-\theta_0)$. Surface diffusion—driven by the local curvature gradients and by the projections of the local electrical field onto the surface—is assumed to exist only at freshly created groove walls in the advancing front. The GB diffusion is driven only by the field. Backstresses in the line are ignored.

The level set simulation enables one to ''capture'' the evolution of the advancing cathode edge surface using realistic, physical boundary conditions. It uses *average* diffusivities, ignoring their orientation dependence. Details are given in Refs. 3 and 4. The model assumes a periodic array of GBs and the computational box shown in Fig. 2 coincides with a single grain (grain 1 in Fig. 1) bound by two GBs. The

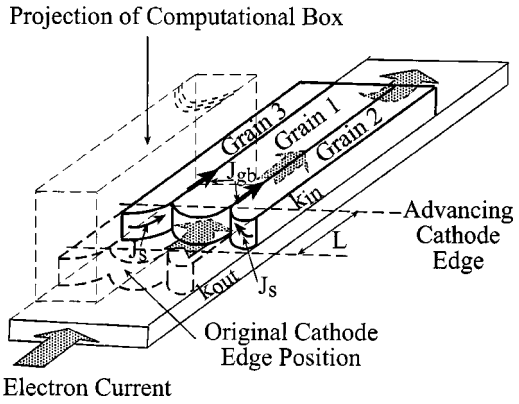

FIG. 1. Schematic description of drift velocity experiment in the idealized geometry used in the simulation, including the projection of the computational box. The cathode edge is scalloped by shallow GB grooves and moves uniformly from left to right under EM. The depth of the groove (relative to the surface maxima) remains constant with time.

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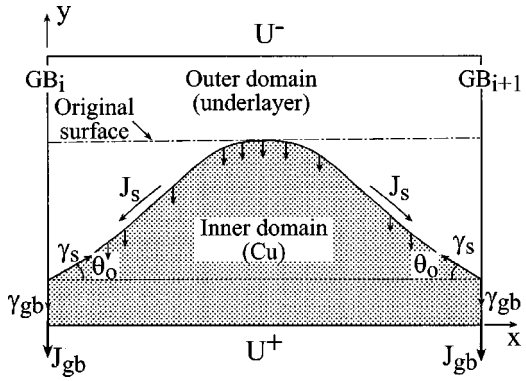

FIG. 2. The computational box, and definitions of various parameters appearing in the simulation. The box contains one grain, its vertical boundaries coinciding with two grain boundaries. The cathode edge moves with time in the $-y$ direction.

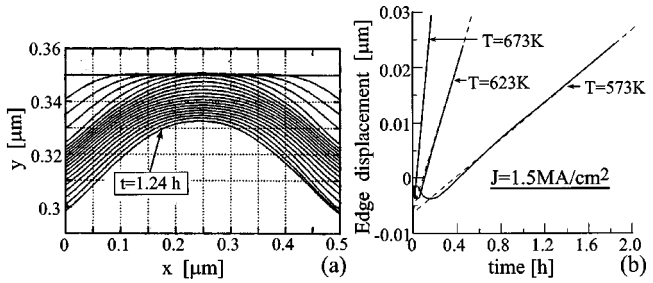

FIG. 3. (a) A series of simulated surface profiles of the advancing cathode edge, dumped every 5000 time steps. The computational box is 0.5 μm $\times 0.5$ μm, and the last profile is dumped after 1.24 h. (b) Distance traveled by the groove tip (triple point) vs time. The tip velocity is approximately equal to the edge velocity, because, as seen in (a), the surface profile remains approximately unchanged with time. The constant slope gives the steady state V_{EM}.

required input parameters are: grain size d, surface and GB diffusivity prefactors $(D_0)_s$ and $(D_0)_{GB}$, and activation energies E_s and E_{GB}, atomic volume Ω, surface and GB widths δ_s and δ_{GB}, surface and GB tensions γ_s and γ_{GB}, electrical conductivities in the grain k_{in} and outside the grain (i.e., in the higher resistivity underlayer, normally a material like Ta, TiN, or TaN) k_{out}, surface and GB effective ionic charges $Z_s = z_s^* e$ and $Z_{GB} = z_{GB}^* e$ where ''e'' is the electron charge, and an electric potential difference $U^+ - U^-$ applied to horizontal boundaries of the computational box (in the drift direction). The original simulation was formulated for constant voltage conditions (constant $U^+ - U^-$). The time-dependent distribution of the electrical field is provided by the solution of the Laplace equation[4] for the electrical potential within the computational box (with Dirichlet boundary conditions prescribed on the horizontal boundaries and Neumann boundary conditions prescribed on the GBs) at every step of time marching. In later simulations, a constant current density j was imposed by adjusting $U^+ - U^-$ after each computational step. Typical simulation results showing the advancing front at equally spaced time steps are shown in Fig. 3(a). The distance traveled by the groove tip is replotted versus time for three temperatures in Fig. 3(b). The steady state V_{EM} is obtained at each T from the constant slope of the lines in Fig. 3(b).

A successful simulation should be able to match the experimental data expressed by Eq. (1) over its entire T range, a ''test'' much more stringent than matching only one velocity at one temperature. In other words, the simulation should generate *both* $(V_0)_{EM}$ and E_{EM} which match the experiments, given realistic and independent (literature) inputs, particularly of $(D_0)_s$, $(D_0)_{GB}$, E_s, and E_{GB}. In addition, it should reproduce known dependencies of V_{EM} on j and d. We calculated the EM drift velocity parameters of pure polycrystalline Cu interconnects, and compared our predictions with the experimental results of Hu *et al.*[2] and Lee *et al.*[7] A typical simulation to obtain one set of $(V_0)_{EM}$ and E_{EM}, run on a 500–600 MHz PC, took about 3 h.

For each input set, V_{EM} was calculated for at least three temperatures in the range 573–723 K, which roughly overlaps the experimental T range in Refs. 2 and 7. The input parameters were: $d = 0.5\,\mu$m, $\Omega = 1.18\times10^{-29}\,\text{m}^3$, $\gamma_s = 1.7\,\text{J/m}^2$, $\gamma_{GB} = 0.6\,\text{J/m}^2$, $\delta_s = \delta_{GB} = 3.5\times10^{-10}\,$m, constant ($T$ independent) $k_{in} = 7.5\times10^6\,(\Omega\,\text{m})^{-1}$ [versus about $20\times10^6\,(\Omega\,\text{m})^{-1}$ used by Hu and about $30\times10^6\,(\Omega\,\text{m})^{-1}$ used by Lee, both at 573 K], $k_{out} = 7.5\times10^5\,(\Omega\,\text{m})^{-1}$, $z_s^* = 0.8$, $z_{GB}^* = 14$ (both taken from Ref. 2) and $U^+ = -U^- = 0.005\,$V over a length of 0.5 μm which translates into a starting $j = 2.7\,\text{MA/cm}^2$. Diffusivity inputs were changed from set to set (except where the effect of other parameter changes was sought). Note that except for the z^* values which are somewhat uncertain (yet derived in Hu's work and generally accepted as of the right order and sign), all others are well-established values accepted in the literature. Under constant U conditions, j drops with time since the length of the low k_{out} section (underlayer) increases, while that of the higher k_{in} (conductor) decreases. The typical value of j at the end of most simulations was about 50%–75% lower than at

TABLE I. Results of constant voltage simulations for three sets of diffusivity input data for pure Cu. The ''experimental values'' of Hu *et al.*[a] were obtained by linear regression from experimental drift velocity values in 5-μm-wide lines in their Fig. 2. The ''experimental'' $(V_0)_{EM}$ in the work of Lee *et al.*[b] was obtained from the reported V_{EM} at 573 K and the reported E_{EM}.

Set No.	Input $(D_0)_{GB}$ ($\times10^{-6}$ m^2/s)	Input E_{GB} (eV)	Input $(D_0)_s$ ($\times10^{-6}$ m^2/s)	Input E_s (eV)	Output $(V_0)_{EM}$ ($\times10^6$ μm/h)	Output E_{EM} (eV)	V_{EM} at 573 K (μm/h)	D_s/D_{GB} at 573 K
1	6	0.95	26	0.90	1.1	0.87	0.02	12
2	6	0.95	15	0.78	1.1	0.84	0.05	77
3	6	0.88	15	0.78	0.9	0.78	0.13	19
Experimental values from Hu *et al.*[a]					4.6	0.94	~0.03	
Experimental values from Lee *et al.*[b]					1.1	0.73	0.08	

[a]See Ref. 2.
[b]See Ref. 7.

TABLE II. Comparison of simulated (using set 1) and experimental drift velocities at different temperatures. Note that in the constant voltage simulation, the current density j drops from about 2.7 to about 1.7 MA/cm^2. The constant j simulation uses $j=1.5$ MA/cm^2. The differences between the two simulations are small.

T (°C)	255	314	370	405	Remarks
Simulation V_{EM} (μm/h)	0.006	0.04	0.18	0.40	Constant V, adjusted for ρ
Simulation V_{EM} (μm/h)	0.006	0.04	0.22	0.55	Constant j, adjusted for ρ
Experimental V_{EM} (μm/h)	0.005	0.05	0.18	0.60	Hu *et al.*[a]

[a]See Ref. 2.

the start. After a short *transient* stage, steady state (constant V_{EM}) was reached in most simulations in about 10 min. From the steady state $V_{EM}(T)$, we extracted $(V_0)_{EM}$ and E_{EM} using linear regression, and then corrected $(V_0)_{EM}$ for the resistivity difference (dividing by 3 for comparison with Hu,[2] and by 4 for comparison with Lee[7]). Input diffusivity and output DV simulation values are listed in Table I, with Hu and Lee's data shown for comparison.

We first used (''set 1'') $(D_0)_s=2.6\times10^{-5}$ m^2/s and $E_s=0.90$ eV, and $(D_0)_{GB}=6\times10^{-6}$ m^2/s and $E_{GB}=0.95$ eV, values referenced in Hu,[2] and derived originally from Surholt and Herzig's[8] and Gupta's[9] studies on Cu GB self-diffusion. The surface diffusivity data originate with Bradshaw *et al.*[10] Uncertainties in these values (both GB and surface diffusivities can be strongly affected by impurities[11]) can materially affect diffusivities at calculation temperatures, but will not impact significantly the conclusions drawn from the simulation results. As shown in Table I, for set 1 inputs, $(V_0)_{EM}=1.1\times10^6$ μm/h and $E_{EM}=0.87$ eV. Input variations were checked with two other sets (sets 2 and 3), one lowering E_s while keeping E_{GB} as in set 1, the other lowering both E_s and E_{GB}. The estimated errors in the simulation results are a factor of 2 in $(V_0)_{EM}$, and less than $\pm5\%$ in E_{EM}.

Experimental $(V_0)_{EM}$ and E_{EM} values were extracted from Fig. 2 in Ref. 2. For a linewidth $w=5$ μm (with d roughly similar to our 0.5 μm), a linear regression gives approximate values of 4.6×10^6 μm/h and 0.94 eV, respectively. The agreement between set 1 simulation results and these values is quite good. An equally good agreement (particularly with set 3 inputs) exists with Ref. 7. There, a measured $V_{EM}=0.08$ μm/h and E_{EM} of 0.73 eV at 300° C is reported for long pure Cu lines and $j=2.1$ MA/cm^2. Use of all their Arrhenius data yields $(V_0)_{EM}=1.1\times10^6$ μm/h. After adjusting for the resistivity difference, set 1 simulations yield $V_{EM}\approx0.02$ μm/h, and set 3 yield $V_{EM}\approx0.1$ μm/h.

A comparison of calculated (using set 1) versus experimental V_{EM} values at the four temperatures of Fig. 2 in Hu's paper are given in Table II. The values are practically identical. The agreement is excellent, particularly in view of the estimated numerical procedure errors, the highly idealized geometry, and the sensitivity of the simulation to the input diffusivity values.

Constant current ($j=1.5$ MA/cm^2) simulations were also performed with set 1 and set 2 parameters. The only input changes, required to ensure simulation stability, were increased k_{in} and k_{out} [to 10^8 and 10^7 $(\Omega\,\mathrm{m})^{-1}$, respectively, resulting in simulation ρ_{Cu} of 1×10^{-8} Ω m, five times lower than Hu's, but only about 3 times lower than Lee's resistivity at 300 C]. The resulting $(V_0)_{EM}$ (after correcting for ρ) and E_{EM} were 2.4×10^6 μm/h and 0.85 eV, respectively, for set 1, and 0.9×10^6 μm/h and 0.75 eV for set 2. The simulation results are again in excellent agreement with the experimental range of Refs. 2 and 7. The calculated V_{EM} at 300° C is now 0.09 μm/h for set 1 and 0.24 μm/h for set 2.

One interesting aspect of this simulation is that it achieves excellent match with experiment while ignoring the role of surfaces and heterogeneous interfaces as alternative EM pathways acting *in parallel* with GBs. Instead, the simulation emphasizes the role of surface diffusion along freshly created groove walls as the coupling process which enables a *homogeneous displacement of the cathode edge*, via redistribution of the ''emptiness'' caused by EM at each GB, over a distance $\sim d$. This clarifies the physics behind the averaging factor δ/d, used traditionally since Blech's[1] work to describe GB EM.

The simulation correctly predicts an inverse dependence of V_{EM} on d,[12] and a direct dependence of V_{EM} on j (albeit weaker than linear, a point to be discussed in detail separately[12]). Clearly, the model assumptions are rather crude, particularly the constrained GB morphology, input uncertainties, the lack of backstress in the line, as well as an explicitly constant J_{GB} (which means that J_s always ''adjusts'' to J_{GB}, while the opposite case of small J_s causing a small J_{GB}, i.e., J_{GB} ''adjusting'' to a given J_s is never considered, a dubious assumption at best[12]).

Nevertheless, this simulation shows that all essential features of homogeneous DV EM in polycrystalline lines can be described in terms of GB grooving, while fulfilling two key continuity and equilibrium conditions, and while accounting for field-driven surface diffusion along freshly created groove walls at the advancing cathode edge.

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