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Letter

An energy approach to predict electromigration induced grain rotation under high current density

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HIGHLIGHTS

- An energy approach is developed to describe the grain rotation in the conducting material under high current density.
- The electric current energy, grain boundary energy, and dissipation energy caused by the diffusion are included in the developed model.
- The proposed model can predict the electromigration induced grain rotation with reasonable accuracy compared with experimental results.

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ABSTRACT

An energy approach is proposed to describe the electromigration induced grain rotation under high current density. The driving force is assumed to arise from the grain-boundary energy reduction and increase of the inner energy from the joule heating. Energy dissipates by the grain boundary diffusion under electromigration and viscous boundary sliding is considered. Based on the conservation of energy production and dissipation, an equilibrium equation is developed to predict the grain rotation rate analytically. It is recognized that the grain rotates with the reducing of electrical resistivity and inversely proportional to the grain length. The theoretical prediction is compared with the experimental data, which shows good accuracy on the rotation trend and the specific rotation rate.

As a representative microstructure evolution phenomenon under high current density in microelectronic interconnects, electromigration induced grain rotation has attracted wide research interest, however, the phenomenon still lacks of reasonable physical interpretation [1-3]. On the other hand, with the miniaturization trend of electronic devices, the diameter of next generation solder interconnect in the advanced three-dimensional electronic packaging has dropped below 50 μm, which may only contain several of grains [4]. Smaller size of interconnect will lead to stronger influence on microstructure of solder interconnect. Therefore, it is essential to understand better the

panied with the mass diffusion. The grain rotation will create volumes where two grains can overlap and leave voids in the other regions. The voids and overlapping regions are mainly caused by the mass diffusion. Harris et al. [5] investigated grain rotation in thin films of gold at high temperature, a kinetics model is proposed based on grain boundary diffusion induced mass transport from the overlapping regions to voids. Moldovan et al. [6] developed a dynamical theory of grain rotation based on the diffusion accommodated grain boundary sliding. Kim et al. [7] established a straight forward energy method to investigate the grain rotation under high current density has been observed experimentally, theoretical analysis is still required to explain this phenomenon. Wu et al. [8, 9] proposed an electromigration induced model based on the mass flux divergence caused by the anisotropic electrical properties of material. The mass flux divergence is assumed to be caused by the bulk diffusion and the grain boundary diffusion is ignored. In addition, the model is one dimensional which limits its application for more complex conditions. A more general theoretical model is still lacking to analyze the electromigration induced grain rotation in solder interconnects.

In the current study, an energy approach is proposed to describe the grain rotation. To avoid the multi physics fields coupling issue, it is assumed that the driving energy is provided by the aggregate grain boundary energy with respect to misorientation and the inner energy increment caused by joule heating effect. The energy is dissipated due to the mass diffusion caused by electromigration and the viscous boundary sliding. As soon as the energy accompanied with the grain rotation is clarified, an energy conservation equation can be developed to determine the grain rotation rate.

As shown in Fig. 1, a regular polygonal grain with n edges is considered with electric current along the horizontal direction. Through geometric operation, the distance r from the grain center to the grain boundary is given by

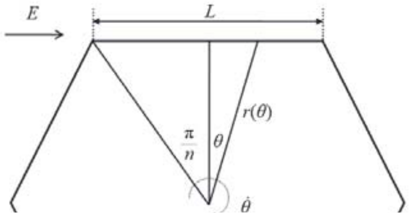
$$r(\theta) = \frac{L}{2\cos\theta\tan(\pi/n)} = \frac{s}{\sin\theta}\,. \tag{1}$$

Due to electromigration, the mass flux on the grain boundary is given by Ref. [10]

$$J = \frac{D_b\,\delta}{\Omega k_{\mathrm{B}} T}\left(-Z^{*}eE\,\cos\vartheta + \Omega\frac{\partial \sigma_n}{\partial s}\right), \tag{2}$$

where D_b is the grain boundary diffusion coefficient. δ represents the thickness of grain boundary. Ω is the atom volume. k_{B} is the Boltzmann's constant. T is the absolute temperature. Z^{*} is the effective charge number. e is the elementary charge. E is the electric field strength. σ_n denotes the normal stress on the grain boundary, which is caused by the coupled effects of electromigration and the grain boundary sliding.

It is recognized that the grain movement is induced by grain boundary diffusion. Based on the mass conversation principle, the normal velocity v_n can be written as



$$v_n = -\Omega\frac{\mathrm{d}J}{\mathrm{d}s}\,. \tag{3}$$

Substituting Eq. (2) into Eq. (3), then we obtain

$$v_n = -\frac{\Omega\delta D}{k_{\mathrm{B}}T}\frac{\mathrm{d}^2\sigma_n}{\mathrm{d}s^2}\,. \tag{4}$$

Denoting the grain rotation rate as $\dot{\theta}$, the normal velocity can be rewritten by the geometrical relationship

$$V_n = r\dot{\theta}\left(\frac{1}{r}\frac{\mathrm{d}r}{\mathrm{d}\theta}\right)\left[1+\left(\frac{1}{r}\frac{\mathrm{d}r}{\mathrm{d}\theta}\right)^2\right]^{-1/2} = s\dot{\theta}. \tag{5}$$

Integral Eqs. (3) and (4) respectively, the relationship between the normal stress and the grain rotation rate can be obtained. The boundary conditions are set as: the total stress on the grain boundary is zero and the stress must be continuous by the ends of the boundary facet. The final normal stress on the grain boundary can be described by

$$\sigma_n = \frac{k_{\mathrm{B}}T\dot{\theta}}{6\Omega\delta D}\left(-s^3 + \frac{L^2 s}{4}\right). \tag{6}$$

Substitute Eq. (6) into Eq. (2), the mass flux on the grain boundary can be rewritten as

$$J = \frac{D\delta}{\Omega k_{\mathrm{B}}T}\left[-Z^{*}eE\,\cos\vartheta + \frac{k_{\mathrm{B}}T\dot{\theta}}{6\delta D}\left(-3s^2 + \frac{L^2}{4}\right)\right]. \tag{7}$$

Denoting v_a as the velocity of the diffusing atoms, v_a is related to the mass flux given by $\Omega J = \delta v_a$, thus

$$v_a = \frac{\Omega J}{\delta} = \frac{D}{k_{\mathrm{B}}T}\left[-Z^{*}eE\,\cos\vartheta + \frac{k_{\mathrm{B}}T\dot{\theta}}{6\delta D}\left(-3s^2 + \frac{L^2}{4}\right)\right]. \tag{8}$$

Based on the Einstein's relationship [11], the diffusing atoms velocity v_a is also related to the driving force acting on the atoms $v_a = FD/(k_{\mathrm{B}}T)$. Thus, the energy-dissipation rate of the atom during diffusion process is given by

$$\dot{q} = Fv_a = \frac{k_{\mathrm{B}}T}{D}v_a^2. \tag{9}$$

The diffusion process is dissipated which will decrease the total system energy, so that the diffusion could not act as the driving force. However, by the joule heating effect, the inner energy in the grain will increase and the atoms become more active, thus, the grain movement trend is rising. Integral Eq. (9)

$$\dot{W}_D = \frac{\delta D}{\Omega k_{\mathrm{B}} T}\left[(Z^* eE \cos\vartheta)^2 L + \left(\frac{k_{\mathrm{B}} T\dot{\theta}}{6\delta D}\right)^2 \frac{L^5}{20}\right]. \tag{11}$$

The above energy dissipation is caused by the normal stress and the electromigration, which plays an important role of altering the chemical potential to drive the atoms diffusion. On the other hand, it is recognized that the grain boundary is accompanied with the grain boundary sliding. Therefore, the corresponding energy-dissipation ($\dot{W}_s$) caused by the shear stress due to the viscous boundary sliding is given by

$$\dot{W}_s = \int \tau_s v_s \mathrm{d}s, \tag{12}$$

where τ_s is the shear stress on the grain boundary and v_s is the tangential component of the relative velocity on the boundary facet. Based on the geometric relationship between the grain rotation and the boundary sliding, the tangential velocity v_s can be obtained

$$v_s = r\dot{\theta}\left[1 + \left(\frac{1}{r}\frac{\mathrm{d}r}{\mathrm{d}\theta}\right)^2\right]^{-1/2} = \frac{L\dot{\theta}}{2\tan(\pi/n)}. \tag{13}$$

Assuming the viscous sliding is described by a Newtonian flow, the shear stress τ_s can be defined as $\eta v_s/\delta$, where η is the viscosity with respect to the boundary sliding. Combining Eq. (12) with Eq. (13), the energy dissipation rate due to the grain boundary sliding is determined as

$$\dot{W}_s = \int \tau_s v_s \mathrm{d}s = \int \frac{\eta}{\delta}\left[\frac{L\dot{\theta}}{2\tan(\pi/n)}\right]^2 \mathrm{d}s = \frac{\eta}{\delta}\left[\frac{L\dot{\theta}}{2\tan(\pi/n)}\right]^2 L. \tag{14}$$

In the steady state, it is recognized that the total energy dissipation by the mass diffusion and boundary sliding, while the energy production is supplied by external work and the grain boundary energy W_G. The energy balance equation is written as

$$\dot{W}_s + \dot{W}_D = \dot{U}_I + \dot{U}_{GB}. \tag{15}$$

It is noted that the external work is mainly done by the electric current. The total energy done by the electric current on a single grain is given by the Joule's Heating law. However, not all the energy has been transformed to the driving energy for grain rotation, some energy is dissipated as heat or causes increasing of the inner energy, and the other part will drive the grain rotation. Denotes χ as the joule heating fraction represents the effective joule heating energy, the external work done by the electric current is given by

$$\dot{U} = \dot{Q} = \chi I^2 R, \tag{16}$$

where R is the electric resistivity of the particular grain.

As the grain rotates, the grain energy will be released to fur-

energy between the grain and its neighbors. $\sum$ represents the summation of all the grain energy around it.

Combining Eqs. (11), (14)-(17), the energy balance equation for the particular grain with n edges can be written as

$$\begin{aligned}&\left[\frac{nk_{\mathrm{B}}T}{720\Omega\delta D}L^5 + n\frac{\eta}{\delta}\frac{L^3}{4\tan^2(\pi/n)}\right]\dot{\theta}^2 - L\sum(\mathrm{d}\gamma_i/\mathrm{d}\theta_i)\dot{\theta}\\&+\frac{\delta D}{\Omega k_{\mathrm{B}}T}(Z^* eE)^2 f(\vartheta)L - \chi I^2 R = 0.\end{aligned} \tag{18}$$

For the rectangle grain with four edges $f(\vartheta) = 2$, and for hexagon grain with six edges $f(\vartheta) = 3$. Equation (18) is a quadratic equation with respect to the grain boundary rate, which can be solved by the extract roots formula. The discriminant for the Eq. (18) is given by

$$\begin{aligned}\varDelta = &\left(L\sum\frac{\mathrm{d}\gamma_i}{\mathrm{d}\theta_i}\right)^2 - 4n\left[\frac{k_{\mathrm{B}}T}{720\Omega\delta D}L^5 + \frac{\eta}{\delta}\frac{L^3}{4\tan^2(\pi/n)}\right]\cdot\\&\left[\frac{\delta D}{\Omega k_{\mathrm{B}}T}(Z^* eE)^2 f(\vartheta)L - \chi I^2 R\right].\end{aligned} \tag{19}$$

As the energy dissipation must be less than the energy production, namely $\frac{\delta D}{\Omega k_{\mathrm{B}}T}(Z^* eE)^2 f(\vartheta)L < \chi I^2 R$, the discriminant $\varDelta > 0$. There exists two roots of Eq. (18) and the one less than zero is ignored. Thus, the grain rotation rate by solving Eq. (18) is given by

$$\dot{\theta} = \frac{\sum\frac{\mathrm{d}\gamma_i}{\mathrm{d}\theta_i} + \sqrt{\varDelta}}{2\left[\frac{nk_{\mathrm{B}}T}{720\Omega\delta D}L^4 + \frac{\eta}{\delta}\frac{nL^2}{4\tan^2(\pi/n)}\right]}. \tag{20}$$

Based on Eq. (20), an analytical formula is proposed to describe the electromigration induced grain rotation under high current density. It is noted that most of the parameters in the equation are available except for the electric resistivity R and joule heating fraction χ. To simply the analysis, a non-dimension electromigration parameter β is defined as

$$\beta = \frac{\chi I^2 R}{\frac{\delta D}{\Omega k_{\mathrm{B}}T}(Z^* eE)^2 f(\vartheta)L}, \tag{21}$$

where β is the energy conversion rate of the electric current and $\beta > 1$. The parameter represents the effect of electromigration on the total electric energy. It is well accepted that the total energy of electric current mainly consists of the joule heating and the diffusion dissipation when it flows into the pure conductor. However, it is not valid to determine the specific parameter by using the traditional approach. A computational analysis should be conducted with molecular dynamic analysis or the first principle method to obtain the beta value numerically

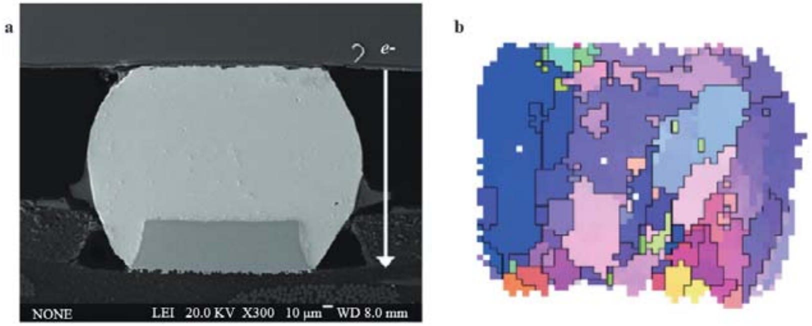


Fig. 2. **a** Schematic diagram of solder joints observed in the scanning electron microscope (SEM), **b** grains distribution map [12].

induced grain rotation phenomenon in the experiments can be explained qualitatively. Based on the analysis, the grain rotation will towards the direction of required minimum energy. This explains why the grains rotate in the trend of reducing the electrical resistivity, as observed in the experiment [12]. On the other hand, the gains with high-angle grain boundaries and smaller size can be easily rotated [3]. Based on the proposed model, the grain rotation rate is proportional to the grain boundary energy and inversely proportional to the grain length L. The grains with high-angle grain boundaries own higher grain boundary energy. Additionally, it is realized that electromigration induced grain rotation is mainly motivated by the inner energy increment by the joule heating effect, while the electromigration will increase the dissipation energy which will restrict the grain rotation. It further proves that the grain rotation occurs at high temperature with thermal activation of the atoms. Considering a case with the viscosity η = 0, meaning that grain can slide at an infinite rate and the grain edges $n = \infty$, the grain becomes a cylindrical rod. The grain length tends to be infinitesimal and the diffusion energy dissipation decreases rapidly, so that the grain will rotate at an infinite velocity. Furthermore, if the electric current effect is ignored, the grain rotation rate is proportional to $1/L^4$, which agrees well with other theoretical analysis [7].

The developed theoretical model is further verified with the experimental results by Shen et al. [12]. In their experiment, the flip chip lead free solder joint (Sn–0.7%Cu) was stressed at an average electric density of 1.25×10^4 A/cm^2 at (75 ± 2)°C for 43 hours. It is found that grain rotation mainly occurs at the current crowding zone. The two grains located at the current crowing zone is rotated with 0.014° and 0.0009° per hour respectively, as shown in Fig. 2. The grain is represented by the hexagon shape and the average grain length ranges from 15 μm to 30 μm. As the component of Cu in the solder joint is relatively small (0.7%), the material parameters of pure Sn are adopted as listed in Table 1.

Up till now, most of the parameters in the developed model are available except for the viscosity η, the electromigration ef-

As for the current crowding and electromigration effect, a case study of these two parameters is conducted based on $\alpha\in(1,10)$ and $\beta\in(1,10)$, the range is of physical significance. The grain boundary diffusion coefficient is chosen as 1.5×10^{-7} cm^2/s to consider the temperature decreasing effect. A range from 0.005 to 0.03 is chosen corresponding to the experimental result. Figure 3 shows the comparison between the theoretical prediction and the experimental data [12] based on the average grain length $L = (15+30)/2 = 22.5$ μm. It is found that the theoretical prediction ranges at the same order of the experimental results. The maximum value from theoretical prediction is about 0.08° per hour when $\alpha = \beta = 10$. For $\alpha = 3$ and $\beta = 5$, generally the theoretical result agrees well with the experimental observations. In summary, the theoretical model with the potential range of the parameters α and β matches the experimental observations with reasonable accuracy.

The parameters α and β are further investigated semi-quantitatively. A coupled thermal-electric finite element model is developed using the same parameters of the experiment [12]. As shown in Fig. 4, an obvious current crowding phenomenon is observed at the corner of solder joint due to the line-to-bump geometry. The average current density in the current crowding zone is about 3–5 times higher than the rest region of the solder interconnect. For a two dimensional case, assuming the grain

Table 1 Material parameter for the pure Sn.

Material parameters	Value
Atom volume Ω (m^3)	2×10^{-29}
Gain boundary thickness (m)	3×10^{-10}
Boltzmann constant k_B (J/K)	1.38×10^{-23}
Effective charge number of pure Sn Z^*	7
Electric resistivity ρ (Ω·m) [13]	13.5×10^{-8}

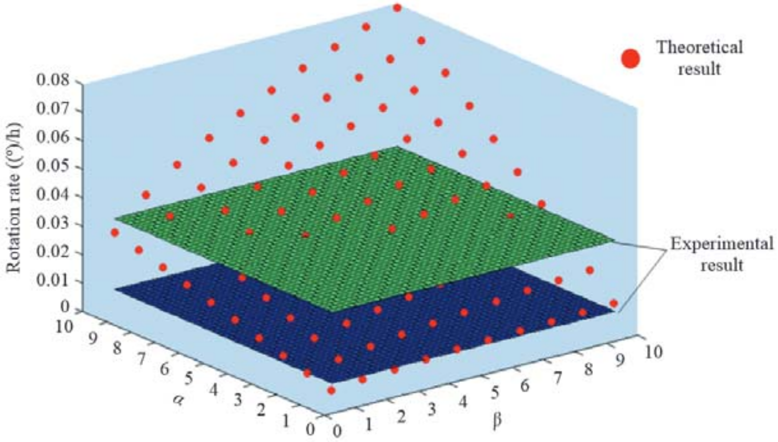


Fig. 3. Comparison of grain rotation rate between the theoretical and experimental results [12] with a grain length of 22.5 μm.

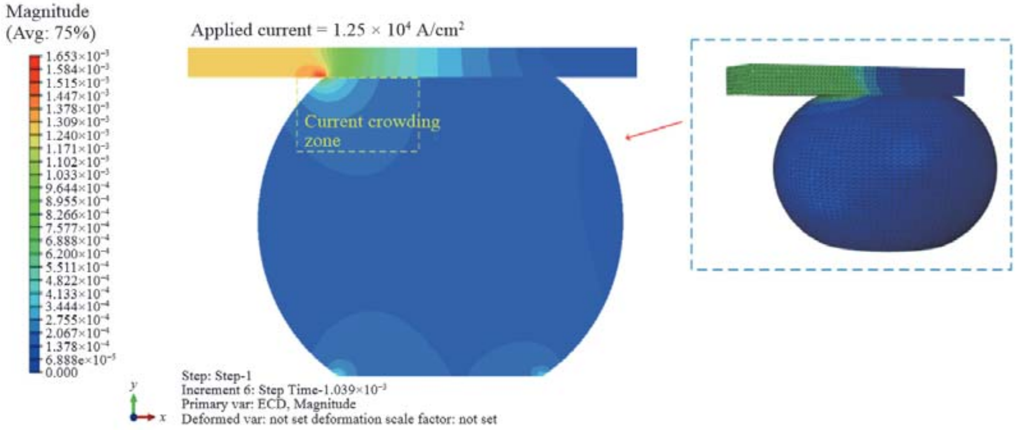


Fig. 4. Current crowding phenomenon in solder joint under high current density due to the line-to-bump geometry.

length $L = 22.5$ μm, the joule heat fraction $\chi = 0.1$ (meaning only 10% of the total electric energy is converted into the inner energy) and the thickness of the grain is 0.1 μm (the ratio between the grain thickness and the length is 1/20), the resultant parameter β is determined as 5.16. When α is from 3 to 5 and β is 5, the theoretical result matches well with the experimental results, as shown in Fig. 3. Particularly, it shows that the parameters range chosen in Fig. 3 is reasonable and coincides with the experiment results.

Based on the theoretical analysis, electromigration diffusion can motivate the grain rotation; however, the process is dissipated by neglecting the anisotropy effect of the electric conductiv-

the flux divergence model can hardly be applied to analyze the grain rotation trend with low electric resistivity.

An energy approach is developed to describe the grain rotation in the conducting polycrystalline material under high current density. The electric current energy, the grain boundary energy and the dissipation energy caused by the diffusion are considered in the developed model. The driving force comes from the reduction of grain boundary energy and the joule heating effect. The rotation process is accompanied with grain-boundary diffusion to keep mass conservation during the rotation process. An energy balance equation is established based on the grain rotation rate and an analytical solution of the electromigration iners.

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