A new model for electromigration grain boundary noise based on free volume*

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Grain boundary plays a key role in electromigration process of polycrystal interconnection. We take a free volume to represent a 'vacancy–ion complex' as a function of grain boundary specific resistivity, and develop a new characterisation model for grain boundary noise. This model reveals the internal relation between the boundary scattering section and electromigration noise. Comparing the simulation result with our experimental result, we find the source as well as the form of noise change in the electromigration process. In order to describe the noise enhancement at grain boundary quantitatively, we propose a new parameter—grain boundary noise enhancement factor, which reflects that the grain boundary noise can characterise the electromigration damage sensitively.

Keywords: free volume, electromigration, grain boundary noise
PACC: 7270, 6630Q, 6170N

1. Introduction

Electromigration in metal film has been a serious problem in interconnection reliability since the critical dimension has attained to ultra-deep submicron.[1,2] As is well known, grain boundaries in polycrystal are not only the fast paths for atoms diffusion, but also mobile defects themselves, through absorbing energy from moving conduction electrons, grain boundaries contribute almost all the resistance in metals.[3] Based on the view above, through analysing the electrons scattering by grain boundaries, Dannenberg *et al.*[3] focused on the study of boundary specific resistivity of metal film, and derived a relationship between electron wind force and specific resistivity in the area of grain boundary. Both simulative and experimental results proved that the electron wind force near grain boundary is 1–2 orders greater than in the bulk in electromigration process.[3−5]

For years, with the durative development in reliability characterisation and estimation, besides some ordinary methods, such as drift velocity analysis,[6] lifetime testing,[7] resistance monitoring,[8] *in-situ* analysis, etc.,[9] noise testing has appeared as a new method of analysing the electromigration damage. Because of its convenient, sensitive and non-destructive capability, noise soon became a hotspot in research. At the present stage, researchers' interests mainly fasten on the comparison between noise and ordinary parameters,[10] or the relationship between noise and failure time, stress, geometry characterisation etc.,[11,12] or noise time–frequency analysis.[13−15] However, there are fewer researches on the relativity between noise and the electromigration dominant defect–grain boundary. Through noise testing for polycrystal interconnections, Ciofi *et al.*[16,17] proved that electromigration mainly takes place at grain boundary. Yang and Butler[18] attributed the $1/f$ noise in metal film to the electron mobility ratio fluctuation caused by vacancy fluctuation at grain boundary. Here, f is the noise frequency. These results inspire us to research the relationship between noise and grain boundary deeply.

Based on the specific resistivity of grain boundary, through the introduction of free volume, we establish a grain boundary noise model. The simulative and the experimental results show that during the early stage of electromigration, noise is in the form of $1/f$, it origins mainly from the scattering caused by the equilibrium exchange of vacancies and atoms in the bulk; along with electromigration process, vacancies gather at grain boundary and form free volume scattering section, the $1/f$ noise turns into $1/f^2$ noise. To quantify

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the enhancement of grain boundary noise, boundary noise enhancement factor is proposed by consulting the form of electron wind force enhancement factor.[3] For regular metal interconnection materials, noise enhancement factor caused by free volume scattering at grain boundary is on the order of 10^4, which is much greater than the electron wind enhancement factor, so noise can characterise the electromigration damage more sensitively than conventional electricity parameters.

2. Model

Grain boundary is a special area, and its long-range disorder results in more defects, where ions have an irregular arrangement and greater freedom for motion. Hence, the grain boundary has a more intense scattering for electrons as shown in Fig. 1. The concept of free volume origining from noncrystalline solid was used to describe the grain boundary,[19] we consider grain boundaries as an array of scatterers in a plane, the scatters are called 'vacancy–ion' complexes, in which the vacancy represents the boundary free volume and the ion is an atom adjacent to the vacancy. Thus, grain boundaries can be pictured as a distribution of missing pockets of jullium in a plane, and the pockets represent the free volume found near the dislocation cores. Associated with each pocket of missing

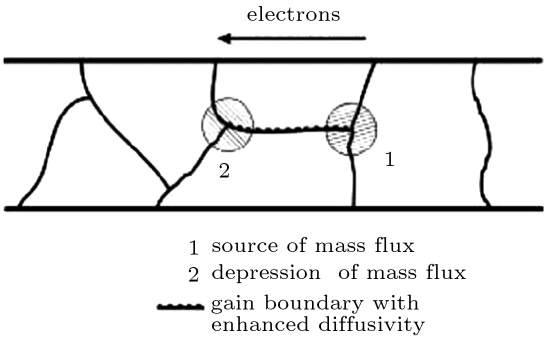


Fig. 1. Sketch of polycrystal grain boundary.

volume is an atom of the metal matrix whose interaction with conduction electrons is stronger than atoms coordinated only by other atoms. This scatter is called a 'vacancy–ion complex'. We assert that the scattering of conduction electrons by atoms of complexes becomes even more prominent than by ordinary atoms.

Based on the view above, several hypotheses are proposed as follows:

(i) grain boundaries are considered as a series of scatterers in a plane;

(ii) the scattering at the grain boundary is due to free volume pockets in the net positive background jellium;

(iii) free volume at grain boundary is a kind of defect in the form of vacancy.

In order to research the relationship between noise and boundary free volume, we should start with grain boundary resistivity. According to Drude expression, boundary resistivity can be written as

$$\rho_{\rm f}(G) = \frac{m}{(n+\delta n)e^2}\omega_{\rm f}(G), \tag{1}$$

where m is the electron effective mass, n is the electron density in the bulk, $n+\delta n$ is the electron density at boundary, e is the electron charge, and $\omega_{\rm f}(G)$ is the scattering probability of free volume. The scatterings are not independent of each other. The specific resistivity of grain boundary can be written as[2]

$$\left[\frac{\Delta\rho}{\Delta\xi}\right] = \rho_{\rm f}(G)\delta = \frac{m}{(n+\delta n)e^2}\omega_{\rm f}(G)\delta, \tag{2}$$

where δ is the width of boundary. The scattering rate at grain boundary is determined by the mean effect of ions with different free volumes. Supposing that $p(v_{\rm f}){\rm d}v_{\rm f}$ is the probability of free volume between $v_{\rm f}$ and $v_{\rm f}+{\rm d}v_{\rm f}$, a method like Maxwell–Boltzmann balance statistics is adopted to obtain the scatterer free volume distribution function as

$$p(v_{\rm f}) = (N_{\rm g}/V_{\rm f})\exp[-(N_{\rm g}/V_{\rm f})v_{\rm f}], \tag{3}$$

where $N_{\rm g}$ represents the ion density at grain boundary, and $V_{\rm f}$ is the total free volume in the polycrystal. Here we consider that the blank of $v_{\rm f}$ tends to minimum, thus $p(v_{\rm f})$ can be seen as a continuous distribution. When the velocity of electron motion is v and the effective scattering sectional area is $S(v_{\rm f})$, the scattering probability can be written as

$$\omega_{\rm f}(G) = \int_0^{V_{\rm f}} vS(v_{\rm f})N_{\rm g}p(v_{\rm f}){\rm d}v_{\rm f} = \int_0^{V_{\rm f}} vS(v_{\rm f})N_{\rm g}(N_{\rm g}/V_{\rm f})\exp(-(N_{\rm g}/V_{\rm f})v_{\rm f}){\rm d}v_{\rm f}. \tag{4}$$

Substituting Eq. (4) into Eq. (2), an expression for boundary specific resistivity can be obtained as

$$\left[\frac{\Delta\rho}{\Delta\xi}\right] = \frac{m\delta}{(n+\delta n)e^2}\int_0^{V_\mathrm{f}} vS(v_\mathrm{f})N_\mathrm{g}(N_\mathrm{g}/V_\mathrm{f})\exp\left(-\frac{N_\mathrm{g}}{V_\mathrm{f}}v_\mathrm{f}\right)\mathrm{d}v_\mathrm{f}$$
$$= \int_0^{V_\mathrm{f}} \frac{m\delta v N_\mathrm{g}^2}{(n+\delta n)e^2 V_\mathrm{f}} S(v_\mathrm{f})\exp\left(-\frac{N_\mathrm{g}v_\mathrm{f}}{V_\mathrm{f}}\right)\mathrm{d}v_\mathrm{f}. \quad (5)$$

Because the change of resistance is caused by the vacancy density change, we consider that the ions adjacent to vacancies are all confined on an ion scale, namely v_f is a finite quantity, so

$$\int_0^{V_\mathrm{f}} \frac{N_\mathrm{g}\exp(-(N_\mathrm{g}/V_\mathrm{f})v_\mathrm{f})}{V_\mathrm{f}}\mathrm{d}v_\mathrm{f} = 1, \quad (6)$$

and

$$\left[\frac{\Delta\rho}{\Delta\xi}\right] = \frac{m\delta v N_\mathrm{g} S(v_\mathrm{f})}{(n+\delta n)e^2}. \quad (7)$$

For different grain boundaries, the value of $N_\mathrm{g}\delta$ can be obtained by simulation, however, for convenience, Dannenberg and King[3] obtained the following relationship through the missing jullium model:

$$N_\mathrm{g}\delta = n_\mathrm{a}\left(\frac{\Delta V}{A}\right), \quad (8)$$

where n_a is the atom density, $(\Delta V/A)$ is the free volume expansion per unit area of grain boundary. Because $(n+\delta n)/n_\mathrm{a} = |Z^*(G)|$ is the effective valence of the ion at grain boundary, Eq. (7) turns into

$$\left[\frac{\Delta\rho}{\Delta\xi}\right] = \frac{mvS(v_\mathrm{f})}{(n+\delta n)e^2}n_\mathrm{a}\left(\frac{\Delta V}{A}\right)$$
$$= \frac{mvS(v_\mathrm{f})}{e^2\,|Z^*(G)|}\left(\frac{\Delta V}{A}\right). \quad (9)$$

Based on the $1/f^\gamma$ noise theory in metal interconnection, the relationship between voltage noise spectrum and resistivity can be written as

$$S_\mathrm{V} = S_\mathrm{R}I^2 = \frac{B}{f^\gamma}\frac{\rho j}{kT}\exp\left(-\frac{E_\mathrm{a}}{kT}\right)I^2, \quad (10)$$

where f is the noise frequency as mentioned above, j is the current density in noise test, k is the Boltzmann constant, T is the noise testing temperature, E_a is the active energy for electromigration, and I is the current in interconnection. Supposing that in the electromigration process, the cross section area of interconnection is S, the voltage noise spectrum of grain boundary should be

$$S_{\mathrm{V}(GB)} = \frac{B}{f^\gamma}\frac{\left[\frac{\Delta\rho}{\Delta\xi}\right]j}{\delta kT}\exp\left(-\frac{E_\mathrm{a}}{kT}\right)(jS)^2$$
$$= \frac{BS^2}{f^\gamma}\frac{mvS(v_\mathrm{f})j^3}{\delta e^2\,|Z^*(G)|\,kT}\left(\frac{\Delta V}{A}\right)$$
$$\times\exp\left(-\frac{E_\mathrm{a}}{kT}\right), \quad (11)$$

where $B = B'NZ^*qD_0$, B' is a constant related to material, N is the density of atoms, Z^*q is the effective ionic charge, $D_0\exp(-E_\mathrm{a}/kT)$ is the diffusivity at grain boundary. There are evidences showing that Eq. (10) holds only for $\gamma \approx 2$,[20] and finally, Eq. (11) turns into

$$S_{\mathrm{V}(GB)} = \frac{B'NZ^*qD_0S^2}{f^2}\frac{mvS(v_\mathrm{f})j^3}{\delta e^2\,|Z^*(G)|\,kT}\left(\frac{\Delta V}{A}\right)$$
$$\times\exp\left(-\frac{E_\mathrm{a}}{kT}\right). \quad (12)$$

3. Discussion

To verify our model, accelerated electromigration testing was performed. The sample was made by a 1 μm standard CMOS technique, which was a standard aluminum interconnection with four pins and plastic dual-in-line package. The sample was 2 μm wide, 1325 μm long, and 0.5 μm thick. Our accelerating conditions were $j = 2\mathrm{MA/cm^2}$ for current stress and $T_\mathrm{A} = 130$ °C for thermal stress. In the accelerated electromigration process, resistance and noise were tested, after 28 hours, the sample failed in the form of open.

Figure 2 shows the change of noise frequency exponent γ in the electromigration process. It can be seen that the electromigration process was divided into three parts by γ: in zone I, $\gamma < 1$ (0 h $\le t <$ 4 h), electromigration damage had not happened yet, we call this period the latent period, the noise originated from the defects introduced by the production technique; in zone II, $1 \le \gamma < 1.5$ (4 h $\le t <$ 16 h) ,noise in this period exhibited a $1/f$ form, under the stress of electron wind, vacancies started to be generated and tended to gather at grain boundary, noise came mainly from the scattering caused by the equilibrium exchange of vacancies and atoms in the bulk; in zone III, $\gamma \ge 1.5$ (16 h $\le t <$ 28 h), vacancies had gathered at grain boundary mostly, boundary scattering became the source of noise, and the $1/f$ noise turned into $1/f^2$ noise.[21]

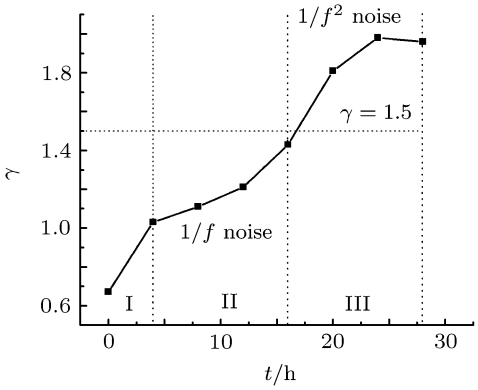


Fig. 2. Variation of noise frequency exponent γ in electromigration process.

Some researchers find that the $1/f^{\gamma}$ noise in metal film originated basically from scattering of carriers by the random movements of impurities and defects, but our noise model describes the $1/f^2$ noise at grain boundary as being induced by free volume. Based on the free volume theory, when vacancies gather at grain boundary to a significant extent, the vacancy–ion complex scattering section will be formed. In the early period after the formation of free volume, its section radius approximates to the ion radius, namely $S(v_{\rm f}) \approx \pi r^2$. According to the analysis above, the noises at two time points, after electromigration had happened, were adopted from zone II and III, and compared with simulation result. For Al interconnection, the parameter values for our noise model are shown in Table 1.

Table 1. Grain boundary noise model parameter values (for Al).

sign	physical meaning	value	reference
$Z^*(G)$	ion effective valence at grain boundary	–456	[3]
T	noise testing temperature/K	300	
$\Delta V/A$	free volume expansion per unit area at grain boundary/cm	$0.05a_0^{\rm Al} = 0.38 \times 10^{-8}$	[3]
$E_{\rm a}$	electromigration active energy/eV	0.6	[22]
r	ionic radius/cm	0.535×10^{-8}	
δ	grain boundary width/cm	10 Å$=1 \times 10^{-7}$	[23]
N	atomic density/cm^{-2}	6×10^6	[24]
Z^*q	effective ionic charge (C)	$15 \times 1.6 \times 10^{-19} = 2.4 \times 10^{-18}$	[25]
$D_0 \exp(-E_{\rm a}/kT)$	diffusivity at grain boundary/(cm^2/s)	6×10^{-13} ($T = 553$ K)	[26]
B'	material constant		

Figure 3 shows the comparison between testing noise and simulation noise. At the early stage of electromigration ($t = 4$ h), the noise was $1/f$ noise, its amplitude was relatively low; at the late stage of electromigration ($t = 20$ h), the noise turned into $1/f^2$ noise and its amplitude increased obviously. The noise at this moment accorded with the simulation result from the free volume model very well, which proves that the $1/f^2$ noise derived from the scattering of free volume at grain boundary indeed, simulation result, agreed with our theoretical prediction also. The scattering section of the simulation result in Fig. 3 was of ionic dimension, and it showed at 20 h the free volume scattering section just formed along with electromigration process. The dimension of scattering section changed constantly until the interconnection failed, and it could develop into the linewidth dimension. Through adjusting the values of terms relevant scattering, such as S, $S(v_{\rm f})$, and $\Delta V/A$, Eq. (12) can still be used to simulate grain boundary noise at any stage of electromigration. Also, through the model, the microcosmic change of grain boundary under electromigration can be obtained simply by noise test.

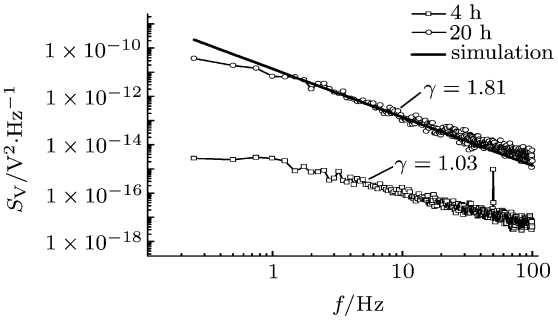


Fig. 3. Comparison between testing noise and simulation noise.

For a polycrystal film, once free volume formed at grain boundary, its scattering for carriers will be more intense than in the bulk, so noise will be enhanced, too (as shown in Fig. 3). In order to quantitatively describe the noise enhancement at grain boundary, referring to the electron wind enhancement factor,[3] we propose a grain boundary noise enhancement factor β

$$\beta = \frac{S_{\rm V}(G)}{S_{\rm V}(\infty)}, \tag{13}$$

where $S_{\rm V}(G)$ is the voltage noise spectrum at grain boundary, and $S_{\rm V}(\infty)$ is the voltage noise spectrum in the bulk under the same stress conditions.

The mass transport during electromigration is attributed to the atom fluxes in grain and at grain boundary. For atom fluxes, the relative contribution of lattice diffusion and boundary diffusion is[23]

$$\frac{J_{1,\rm met}}{J_{\rm b,met}} = \frac{N_{1,\rm met} d_{\rm ave,met} D_{1,\rm met} Z^*_{1,\rm met}}{N_{\rm b,,met} w_{\rm b,met} D_{\rm b,met} Z^*_{\rm b,met}}, \tag{14}$$

where $J_{1,\rm met}$ is the atom stream density in grain, $J_{\rm b,met}$ is the atom stream density at grain boundary, $N_{1,\rm met}$ is the lattice atom density, $N_{\rm b,met}$ is the boundary atom density, $d_{\rm ave,met}$ is the average grain size, $w_{\rm b,met}$ is the effective boundary width, $D_{1,\rm met}$ is the lattice diffusion coefficient, $D_{\rm b,met}$ is the boundary diffusion coefficient, $Z^*_{1,\rm met}$ is the effective ionic charge in lattice, and $Z^*_{\rm b,met}$ is the effective ionic charge at grain boundary. A basic hypothesis for $1/f^\gamma$ noise is that the spectrum density of resistance fluctuation is proportional to atom stream density J, namely $S_{\rm r}(J,f) = CJ/f^\gamma$, according to Eqs. (9) and (14), the noise enhancement factor can be written as

$$\begin{aligned}\beta = \frac{S_{\rm V}(G)}{S_{\rm V}(\infty)} &= C' \frac{J_{\rm b,met}}{J_{1,\rm met}} \\ &= C' \frac{N_{\rm b,met} w_{\rm b,met} D_{\rm b,met} Z^*_{\rm b,met}}{N_{1,\rm met} d_{\rm ave,met} D_{1,\rm met} Z^*_{1,\rm met}}. \end{aligned} \tag{15}$$

For metal films, β is influenced by temperature: for example, when $T = 0.5T_{\rm m,cond}$ ($T_{\rm m,cond}$ denotes the melting temperature), there are[23]

$$\begin{aligned} &\frac{Z^*_{\rm b,met}}{Z^*_{1,\rm met}} \approx 1, \quad \frac{N_{\rm b,met}}{N_{1,\rm met}} \approx 1, \\ &\frac{w_{\rm b,met}}{d_{\rm ave,met}} \approx 10^{-3}, \quad \frac{D_{\rm b,met}}{D_{1,\rm met}} \approx 10^7, \end{aligned} \tag{16}$$

therefore $\beta \approx 10^4$. Comparing the 1–2 order enhancement of electron wind force, the enhancement of noise at grain boundary is remarkable.

4. Conclusion

In this paper the free volume is taken to characterise the noise of polycrystal electromigration, the experimental results verifies the rationality of 'vacancy–ion complex' hypothesis. The grain boundary noise model can be used not only to explain the origin of grain boundary noise but also to make it possible that the microcosmic change and damage of interconnection can be discovered without expensive *in-situ* testing. As an extension for noise characterisation, the grain boundary noise enhancement factor is proposed for the first time, and it validates the close relationship between grain boundary and electromigration noise again. How to make it practical should be our next work.

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