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Electromigration in stressed thin films

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Multilayered thin-film circuits in microelectronic devices are confined in dielectrics for insulation between layers. The confinement produces mechanical stress in the circuit. During operation, the stress can enhance or retard electromigration. This interaction has been analyzed using thermodynamics of irreversible processes and the result applied to short-stripe electromigration experiments. It is shown that the calculated critical length of Al stripes, below which no electromigration damage occurs, agrees well with observation. The critical length is temperature insensitive and allows the effective electromigration-charge number to be determined independently, uncoupled to the diffusivity. In the analysis, a simple expression is given for calculating the effective electromigration-charge number of nearly-free-electron metals on the basis of the ballistic model of scattering.

I. INTRODUCTION

Electromigration is a coerced mass flow in a circuit driven by a direct current when the current density is high, around 10^5 A/cm^2. It is a subject of serious concern in microelectronics because of the reliability failure of interconnecting lines.[1-3] As device miniaturization needs a multilayered structure of metallization to increase circuit density on semiconductor chips, the layered conducting lines which are embedded in dielectrics are subject to stresses. The stress comes from thermal mismatch between the dielectrics such as SiO_2 and the metal such as Al. A stressed metal film tends to relax by creep.[4] Under an applied electrical field, the atomic motion in the stressed film is driven simultaneously by electrical and mechanical forces. Since these forces are directional and their rates of response (the electromigration rate and creep rate) are comparable, they interfere with each other. Owing to the fact that the stress can be tensile or compressive, the interference can enhance or retard electromigration. The interference is analyzed here using the thermodynamics of irreversible processes.[5,6]

II. BACK STRESS IN ELECTROMIGRATION

The effect of stress on electromigration has been observed in the stripe experiment by Blech[7] as depicted in Fig. 1, where a short Al line was deposited on a TiN line on an insulating substrate. The electrical current makes a detour from the TiN to the Al because the latter is a path of lower resistance. At the passage of a high current density, depletion of Al at the cathode end and extrusion of Al at the anode end occur. The morphological changes are due to electromigration. The direction of mass flow in the Al is the same as the flow of electrons.

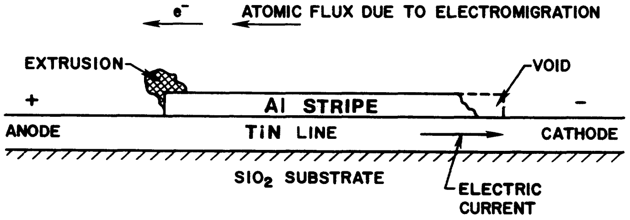

FIG. 1. A sketch of the cross-sectional view of morphological changes due to electromigration in a short Al stripe deposited on a long TiN line.

Specifically, Al stripes of length of 10, 20, 40, and 85 μm were tested at 3.7×10^5 A/cm^2 and 350 °C. After 15 h, all stripes showed damage due to electromigration except the shortest one.[7] In addition, the longer the stripe, the greater the damage. The observation was explained by the counteraction against electromigration from a back stress.[8] Electromigration pushes atoms to the anode and builds up a compressive stress there. The vacancy concentration in the anode becomes less than the equilibrium vacancy concentration according to the Nabarro-Herring model of point-defect formation in a stressed solid.[4] Hence a gradient of vacancy concentration exists in the stripe and the gradient increases with decreasing stripe length. The direction of the gradient is such that it acts against the atomic flux of electromigration, and its magnitude can be large enough to stop electromigration in a very short stripe.

III. IRREVERSIBLE PROCESSES AND DRIVING FORCES

The joint effect of electrical and mechanical forces on mass and current transports in a pure metal is analyzed by a pair of flux equations,[5,6]

$$J_1=L_{11}X_1+L_{12}X_2\ , \tag{1a}$$

$$J_2=L_{21}X_1+L_{22}X_2\ , \tag{1b}$$

where J_1 is the flux of atoms and J_2 is the flux of carriers; $X_1=-\nabla\mu$ is the mechanical force represented by the chemical potential gradient in a stressed solid and $X_2=-\nabla\phi$ is the electrical force represented by the applied electrical field $\mathcal{E}=-\nabla\phi$; and L_{ij} are the linear phenomenological coefficients. L_{11} represents the atomic motion in creep under a normal stress (e.g., pressure) without electrical field. L_{22} is the conductivity of a normal metal without stress. L_{12} and L_{21} are coefficients of the interference terms; in particular, L_{12} is responsible for electromigration and L_{21} for deformation potential (as in a piezoelectric solid under compression, for example). In the following, we shall first discuss the forces, then the coefficients.

For the mechanical force, we consider a thermodynamic process at constant temperature T,[9]

$$p=\left[\frac{\partial F}{\partial V}\right]_T , \tag{2}$$

where p and V are pressure and volume, respectively, and F is Helmholtz free energy. We regard the pressure as an energy density, so the change of energy in an atomic volume Ω is

$$p\Omega=\left[\frac{\partial F}{\partial\left[\dfrac{V}{\Omega}\right]}\right]_T=\left[\frac{\partial F}{\partial N}\right]_T , \tag{3}$$

where $N=V/\Omega$ and $p\Omega$ is by definition the chemical potential in a solid under pressure (or $\sigma\Omega$ under a normal stress σ). So the driving force[4]

$$X_1=-\nabla\sigma\Omega . \tag{4}$$

For the electrical force, $X_2=\mathcal{E}$. The corresponding force on an electron and an ion are $e\mathcal{E}$ and $Z^*e\mathcal{E}$, respectively. Z^* is called the effective charge number of an ion in electromigration and consists of two parts,[10–13]

$$Z^*=Z^*_{el}+Z^*_{wd} , \tag{5}$$

where Z^*_{el} can be regarded as the nominal valence (Z) of the metal when the dynamical screening effect around the ion is ignored and is responsible for the field effect, and $Z^*_{el}e\mathcal{E}$ is often called the "direct force"; and Z^*_{wd} represents the momentum exchange effect between the carriers and the ion, and $Z^*_{wd}e\mathcal{E}$ is commonly called the "electron wind force" in metals.

To envisage the electron wind force, Fig. 2 depicts the configuration of a shaded atom and a neighboring vacancy in a face-centered-cubic structure initially and at the midpoint of exchanging their positions along a $\langle 110\rangle$ direction. The pair have four nearest-neighbors in common, including the two shown by the dashed circles, one on top and one on the bottom of the close-packed atomic plane as shown in Fig. 2(a). At the midpoint of diffusing towards the vacancy, the shaded atom sits on the saddle point as shown in Fig. 2(b) and it is out of the lattice periodicity. Hence it imposes a stronger resistance to electrical current than a normal atom, in other words, it experiences a greater electron scattering or a greater electron wind force. The diffusion of the atom is found to be enhanced in the direction of the electron flow, so the momentum exchange effect is much greater than the electrostatic field effect for electromigration in metals. Z^*_{wd} has generally been measured to be of the order of 10 for nearly-free-electron metals such as Al.

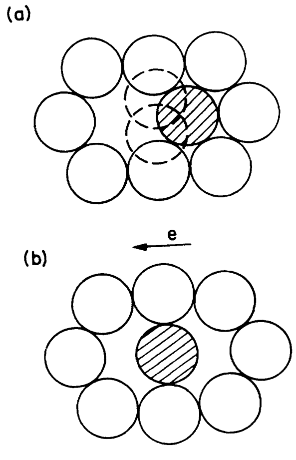

FIG. 2. A sketch of the diffusion of the shaded atom to a neighboring vacancy. The pair have four nearest neighbors in common, including the two drawn in dashed circles (a) before diffusion, and (b) midway during diffusion.

Using a semiclassical ballistic model of scattering, Huntington and Grone[11] obtained an expression of Z^*_{wd} in terms of a specific resistivity ratio

$$Z^*_{wd}=-Z\frac{\dfrac{\rho_d}{N_d}}{\dfrac{\rho}{N}}\frac{m_0}{m^*} , \tag{6}$$

where ρ_d/N_d and ρ/N are specific resistivity of a diffusing atom and a normal atom, respectively, and m_0 and m^* are the free-electron mass and effective electron mass, respectively. There have been several attempts to use quantum-mechanical treatments[14–18] for refining the scattering of the diffusing atom and its surroundings. A recent review of these treatments has been given by Verbruggen.[19] It will not be repeated here and for the purpose of the present analysis the result of the ballistic model is used.

If the specific resistivity of an atom in a metal is assumed to be proportional to the elastic cross section of scattering, which in turn is assumed to be proportional to the average square displacement from equilibrium, or $\langle x^2\rangle$, the cross section of a normal atom can be estimated from the Einstein model of atomic vibration in which the energy of each mode is

$$\tfrac{1}{2}m\omega^2\langle x^2\rangle=\tfrac{1}{2}kT , \tag{7}$$

where the product $m\omega^2$ is the force constant of the vibration, and m and ω are atomic mass and angular vibrational frequency, respectively.

To obtain the cross section of scattering of the diffusing atom, $\langle x_d^2\rangle$, we assume that the atom and its surrounding as shown in Fig. 2(b) have acquired the motion energy of diffusion, ΔH_m, which is independent of temperature,

$$\tfrac{1}{2}m\omega^2\langle x_d^2\rangle=\Delta H_m . \tag{8}$$

Then the ratio of Eq. (7) to Eq. (8) gives the ratio of cross

TABLE I. Comparison of the measured and calculated values of Z^*. Data of measured Z^* taken from Huntington (Ref. 13), where the correlation factor is ignored. Data of ΔH_m taken from Gupta (Ref. 20).

Metal	Measured Z^*	Temp (°C)	ΔH_m (eV)	Calculated Z^*
Monovalent				
Au	−9.5 to −7.5	850 to 1000	0.83	−7.6 to −6.6
Ag	−8.3±1.8	795 to 900	0.66	−6.2 to −5.5
Cu	−4.8±1.5	870 to 1005	0.71	−6.3 to −5.4
Trivalent				
Al	−30 to −12	480 to 640	0.62	−25.6 to −20.6
Quadrivalent				
Pb	−47	250	0.54	−44

section of scattering,

$$\frac{\langle x_d^2\rangle}{\langle x^2\rangle}=\frac{2\,\Delta H_m}{kT}\ . \tag{9}$$

It shows that the ratio varies inversely with temperature. This dependence comes from Eq. (7) which bears the well-known fact that the resistivity of a normal metal varies linearly with temperature above Debye temperature. Substituting Eq. (9) into Eq. (6), combined with Eq. (5), we have

$$Z^*=-Z\left[\frac{\Delta H_m}{kT}\frac{m_0}{m^*}-1\right]\ . \tag{10}$$

In Eq. (10), the numerical factor of $\frac{1}{2}$ has been canceled when the probability of averaging jumps in a given direction (i.e., the direction of electron flow) from among the 12 $\langle 110\rangle$ paths in a fcc lattice is taken into account. Since ΔH_m for most of the fcc metals has been measured,[20,21] we can calculate Z^* at a given temperature by using Eq. (10). The calculated values of Z^* using Eq. (10) agree quite well with those measured for Au, Ag, Cu, Al, and Pb, see Table I. For example, at 480 °C, the measured and calculated Z^* for Al ($\Delta H_m=0.62$ eV) are about −30 and −26, respectively. The temperature dependence of Z^* calculated for Au is also found to agree well with the measured values; see Fig. 3.

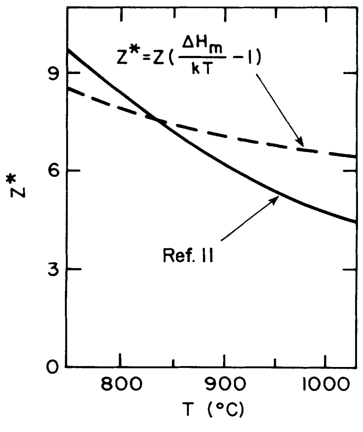

FIG. 3. Plot of Z^* against T for electromigration in Au.

IV. THE PHENOMENOLOGICAL COEFFICIENTS

In essence, the phenomenological coefficients in the flux equations consist of a concentration term and a mobility term. We rewrite Eq. (1) as

$$J_m=-N\frac{D}{kT}\nabla\sigma\Omega-N\frac{D}{kT}Z^*e\nabla\phi\ , \tag{11a}$$

$$J_e=-ne\mu_e N^*\nabla\sigma\Omega-ne\mu_e\nabla\phi\ . \tag{11b}$$

In the equation for J_m (flux of atoms in units of atoms/cm^2 sec), N is concentration of atoms per unit volume, D/kT is atomic mobility with D being the diffusivity. The first term in J_m is known as the creep term and the second term the electromigration term. In the equation for J_e (flux of electrons in units of C/cm^2 sec), the second term describes the conduction of a normal metal and $(ne\mu_e)^{-1}=\rho$ is resistivity in which $n=NZ$ is the number of conduction electrons per unit volume, e is the electron charge, and so ne is the concentration of charges per unit volume, and μ_e is electron mobility. The first term has a parameter N^* which will be discussed later.

If we limit our consideration to the x direction and let $J_m=0$ in Eq. (11a), we have

$$\Delta x=\frac{-\Delta\sigma\Omega}{Z^*e\mathscr{E}_x}\ , \tag{12}$$

where $\mathscr{E}_x$ is the component of electrical field in the x direction. If we assume that the stress gradient is linear in the stripe, Eq. (12) presents the critical length which has been given by Blech and Herring[8] to show no electromigration damage in their experiment.

If we consider a short stripe of metal deposited on an insulating substrate and let $J_e=0$ in Eq. (11b), we have

$$N^*=-\frac{1}{\Omega}\left[\frac{d\phi}{d\sigma}\right]_{J_e=0}\ , \tag{13}$$

where $(d\phi/d\sigma)_{J_e=0}$ is deformation potential defined as the electrical potential difference per unit stress difference with zero current. By using Onsager's reciprocity relation, $L_{12}=L_{21}$, we obtain the expression of

$$\left[\frac{d\phi}{d\sigma}\right]_{J_e=0}=\frac{-Z^*D\rho e}{kT}\ . \tag{14}$$

The dimensions of $(d\phi/d\sigma)_{J_e=0}$ and N^* are cm^3/C and C^{-1}, respectively.

V. DISCUSSION

A. Measurement of the critical length

We use Eq. (12) to calculate Δx of Al stripes. If we assume that the extrusion at the anode is accompanied by a certain amount of plastic deformation, the stress change is taken to be the value corresponding to the elastic limit. In fact, the stress measured by Blech and Herring[8] was very close to the elastic limit value. So the compressive stress $\sigma_{\mathrm{Al}}=-1.2\times10^{9}$ dyn/cm^2; $\Omega_{\mathrm{Al}}=16\times10^{-24}$ cm^3; $e=1.6\times10^{-19}$ C; and $\mathcal{E}_x=J_e\rho=1.54$ V/cm where $J_e=3.7\times10^{5}$ A/cm^2 and $\rho_{\mathrm{Al}}=4.15\times10^{-6}$ Ω cm at 350 °C. Substituting these values into Eq. (12), we obtain

$$\Delta x_{\mathrm{Al}}=\frac{-78\ \mu\mathrm{m}}{Z^*}\ .$$

By taking $Z^*=-26$ for bulk Al, we have $\Delta x_{\mathrm{Al}}=3$ μm, which is of the right order of magnitude, yet shorter than the experimental value found in between 10 and 20 μm.[7] Since the Al stripes are polycrystalline thin films, grain-boundary diffusion might have played a dominant role in electromigration and Z^* for atoms diffusing in grain boundaries might be different from those in the lattice. It seems that for the polycrystalline Al thin films, Z^* lies in the range of 4–8.

Note that the critical length can be measured experimentally by extending the time of electromigration to a sufficiently long period until the mass transport in the strip ceases. An interesting question about the measurement is whether Δx depends on temperature or not.

The temperature dependence of Δx can be examined by substituting Eq. (10) and $\mathcal{E}_x=J_e\rho$ into Eq. (12); we have

$$\Delta x=\frac{\Delta\sigma\Omega}{-Z\left[\dfrac{\Delta H_m}{kT}\dfrac{m_0}{m^*}-1\right]eJ_e\rho}\ . \qquad (15)$$

For normal metals whose electrical resistivity increases linearly with temperature above Debye temperature, Eq. (15) shows that Δx is rather insensitive to temperature provided Z^* of the stripe obeys Eq. (10) and $\Delta H_m \gg kT$. This means that it applies to single crystal stripes or those stripes having grains larger than the width of the stripe. For fine-grained polycrystalline thin films, the temperature dependence of Δx is influenced by the temperature dependence of Z^*.

B. Measurement of the effective charge number

Rearranging Eq. (12), we have

$$Z^*=\frac{-\Delta\sigma\Omega}{\Delta x e\mathcal{E}_x}\ . \qquad (16)$$

It shows that we can calculate Z^* by measuring Δx and $\Delta\sigma$. The latter can be determined by x-ray diffraction of the change in lattice parameter between the ends of the stripe. The advantage of using Eq. (16) for Z^* measurement is that it determines Z^* alone rather than a product of Z^* and another parameter. This is because the other conventional methods of determining electromigration in a pure metal measure either the amount of mass transport or the drift velocity and render a product of Z^* and D.[1–3,13] To separate them an independent measurement of the diffusivity is required. Equation (16) enables the product of DZ^* to be checked by knowing Z^* and D independently.

At present, very little is known about the effective charge number of grain-boundary electromigration. The difficulty of measuring the Z^* which corresponds to grain-boundary diffusion is linked to the lack of understanding of the atomistic mechanism of grain-boundary diffusion. In turn it becomes difficult to separate out the effective charge number from grain-boundary diffusivity if the latter is not known accurately. Since electromigration in thin films is technologically important, a systematic measure of Z^* in polycrystalline thin films as a function of microstructure, composition, and temperature is of interest. Knowing the effective charge number of grain-boundary electromigration, we might use Eq. (10) to investigate the motion energy of grain-boundary diffusion and grain-boundary creep.

C. Measurement of the deformation potential

To calculate $(d\phi/d\sigma)_{J_e=0}$ of Eq. (14), we take $Z^*=-26$ for Al at $T=500$ °C, $kT=0.067$ eV, lattice diffusivity of Al to be about 2×10^{-10} cm^2/sec, and resistivity about 4.83×10^{-6} Ω cm, and we obtain

$$\left[\frac{d\phi}{d\sigma}\right]_{J_e=0}=3.7\times10^{-13}\ \mathrm{cm}^3/\mathrm{C}\ .$$

However, we expect the order of magnitude of deformation potential to be close to Ω/e, which is 10^{-4} cm^3/C or 10^{-10} V/N m^{-2}. It seems what we have calculated on the basis of Eq. (14) is too small. This is because the deformation involved in Eq. (14) is by creep which depends on long-range atomic diffusion and is a very slow process. On the other hand, the mechanical deformation in the usual sense does not involve thermally activated atomic diffusion, rather the atomic displacement under stress proceeds by the acoustic mode of motion, i.e., at the speed of sound which equals $a_0\nu$, where $a_0=3\times10^{-8}$ cm is an interatomic distance and $\nu=10^{13}$ sec^{-1} is an atomic vibrational frequency. Then, in Eq. (14) if we take $D=a_0^2\nu$ we have

$$\left[\frac{d\phi}{d\sigma}\right]_{J_e=0}=0.2\times10^{-4}\ \mathrm{cm}^3/\mathrm{C}\ ,$$

which is of the expected order of magnitude. Hence the deformation potential due to creep is indeed very small. This is also true for electromigration as implied by Onsager's reciprocity relation; electromigration is negligible in a household extension cord.

D. Criterion of the linear flux equations

To use the linear equations in Eq. (11), we should examine the experimental conditions and check if the criterion of linearity is fulfilled. We consider the atomic flux equation and the driving force of stress, where the linear criterion is[5,6]

$$\frac{a_0 X_1}{kT} \ll 1 \tag{17}$$

and $X_1 = -\partial\sigma\Omega/\partial x$. In general, the stress gradient is small in a long line, yet we shall take the extreme case in which the length is the critical length and the stress is at the elastic limit. We estimate that $a_0 X_1/kT \cong 10^{-5}$ at 500 °C, so the linear criterion is satisfied and the nonlinear effect is insignificant. Similarly, the experimental condition of the electrical field is about 1 V/cm, which is not high, so again the linear criterion is satisfied.

VI. CONCLUSION

Thermodynamics of irreversible processes has been used to analyze electromigration in stressed thin films. The interference between electromigration and creep in short stripes has been examined. The calculated and observed critical lengths of Al stripes agree well with each other. The critical length is found to be temperature insensitive and can be used to determine the effective charge number independent of diffusivity.

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[1] F. M. d'Heurle and R. Rosenberg, *Physics of Thin Films* (Academic, New York, 1973).

[2] F. M. d'Heurle and P. S. Ho, in *Thin Films: Interdiffusion and Reactions,* edited by J. M. Poate, K. N. Tu, and J. W. Mayer (Wiley-Interscience, New York, 1978).

[3] P. S. Ho and T. Kwok, Rep. Prog. Phys. **52**, 301 (1989).

[4] C. Herring, J. Appl. Phys. **21**, 437 (1950).

[5] I. Prigogine, *Introduction to Thermodynamics of Irreversible Processes,* 3rd ed. (Wiley-Interscience, New York, 1967).

[6] S. R. de Groot and P. Mazur, *Non-Equilibrium Thermodynamics* (Dover, New York, 1984).

[7] I. A. Blech, J. Appl. Phys. **47**, 1203 (1976).

[8] I. A. Blech and C. Herring, Appl. Phys. Lett. **29**, 131 (1976).

[9] A. B. Pippard, *The Elements of Classical Thermodynamics* (Cambridge University Press, Cambridge, 1966).

[10] V. B. Fiks, Fiz. Tverd. Tela (Leningrad) **1**, 16 (1959) [Sov. Phys. Solid State **1**, 14 (1959)].

[11] H. B. Huntington and A. R. Grone, J. Phys. Chem. Solids **20**, 76 (1961).

[12] H. B. Huntington, in *Low Temperature Diffusion and Applications to Thin Films,* edited by A. Gangulee, P. S. Ho, and K. N. Tu (Elsevier Sequoia, Lausanne, 1975).

[13] H. B. Huntington, in *Diffusion in Solids: Recent Developments,* edited by A. S. Nowick and J. J. Burton (Academic, New York, 1974).

[14] C. Bosvieux and J. Friedel, J. Phys. Chem. Solids **23**, 123 (1962).

[15] R. Landauer, Phys. Rev. B **14**, 1474 (1976).

[16] R. Landauer and J. W. F. Woo, Phys. Rev. B **10**, 1266 (1974).

[17] R. S. Sorbello, J. Phys. Chem. Solids **34**, 937 (1973).

[18] R. S. Sorbello, Phys. Rev. B **31**, 798 (1985).

[19] A. Verbruggen, IBM J. Res. Dev. **32**, 93 (1988).

[20] D. Gupta, in *Diffusion Phenomena in Thin Films and Microelectronic Materials,* edited by D. Gupta and P. S. Ho (Noyes, Park Ridge, NJ, 1988).

[21] P. G. Shewmon, *Diffusion in Solids,* 2nd ed. (The Minerals, Metals and Materials Society, Warrendale, PA, 1989).