PHYSICS OF ELECTROMIGRATION

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Summary

This survey paper on electromigration describes factors which govern the rate of electromigration and therefore relate to the lifetime of conductors stressed at high current density. These include the type of metal conductor, the conductor cross sectional area, lattice, grain boundary and surface diffusion effects, the addition of alloying elements, temperature and current density as well as the thermal conductivity of the substrate. The effect of gradients in temperature, current density, conductor composition and grain size on conductor lifetime are also discussed.

Introduction

The phenomenon of electromigration has been recognized as a potential semiconductor device wear-out failure mode for the past eight or nine years. Although many papers have been published describing reliability data obtained from electromigration studies it is believed that many electronic device reliability engineers do not have a good understanding of the processes involved. It is the purpose of this paper to describe those processes which promote and modify electromigration to enable electronic and electrical engineers to better understand this potential failure mechanism.

Structure of Metal

A metal crystal can be defined as an orderly array of an aggregate of metal ions which are bound together by forces resulting from the ions sharing their valence electrons with the entire aggregate. The degree to which the ions are pulled together by the binding force is opposed by the mutual repulsion of the ions and their associated closed electron shells. Thus each atom in the three dimensional array can be considered to be in a potential well in which it can thermally vibrate with an assignable mean frequency and only through very short distances. The vibrations continually change in amplitude and in direction.

Figure 1 is intended to depict two adjacent ions in a large three dimensional array oscillating in their potential wells. The temperature of a material corresponds to the mean kinetic energy of thermal agitation of the atoms of that material. The value of the mean kinetic energy is 1/2 kT for each degree of freedom of the atom, there k is Boltzmann's constant and T is the absolute temperature. As the metal ions roll back and forth within their potential wells (vibrate) they continuously exchange their energy between potential energy and kinetic energy. When at the bottom of the well the energy is purely kinetic and equal to kT while at the maximum height up the well the energy is purely potential and is also equal to kT. The average values of the potential and kinetic energies are each 1/2 kT.

Figure 2 shows the actual values of the kinetic energy of the ions at a given instant are distributed accordingly to the Boltzmann distribution. This distribution leads to the result that a portion, p, of atoms having a kinetic energy in excess of any particular value Q is given by $p = \exp(-Q/kT)$. The temperature determines what proportion of atoms at any instant have an energy greater than a given value.

Self Diffusion

At any temperature other than absolute zero there is always a percentage of metal ions within the crystalline lattice that possess sufficient energy to escape from the potential well which binds them in the lattice. These ions, when they reach the saddle point of the potential well, where they are essentially free of the lattice and are free to diffuse out or fall back into the well, are termed "activated." As we have seen above, the number of ions which are activated increases exponentially with increasing temperature. The process of diffusion of the ions within their own lattice is termed "self diffusion" and is a random rearrangement of the individual ions which takes place under no concentration gradient or chemical potential and therefore results in no net mass transport.

Self diffusion in close spaced crystalline arrays of ions (such as the face centered cubic structure of aluminum) takes place by an ion exchange with a near neighbor vacancy. See Figure 3. Thus the activation energy for self diffusion of aluminum takes place in two steps. One involves the activation energy for vacancy formation E_f and determines the density of lattice sites that are vacant at a given instant as a function of temperature. The second part involves the activation energy, E_j, for the near neighbor ion-vacancy jump process and determines the number of lattice sites that energetically could make the exchange as a function of temperature. The sum of these energies gives the activation energy for self diffusion, Q. By heating and quenching studies of bulk aluminum it has been determined that $E_f = 0.73$ eV and $E_j = 0.75$ eV thus $Q = E_f + E_j = 1.48$ eV[1]. This is the activation energy for self diffusion of aluminum ions through the crystalline lattice. Each jump takes place in a direction that is independent of the direction of the previous jump and takes place in a random fashion in the crystal structure in directions towards anyone of the 12 possible nearest neighbor vacancies.

Electromigration

Electromigration is the transport of ions through a conductor resulting from the passage of direct current. It is caused by a modification of self diffusion from a random process to a directional one by the presence of an electric field and charge carrier flow.

A metal ion in a current carrying conductor is subjected to two forces. One force (F_E) is due to the positive ion interaction with an electric field and is in the direction of that field. The second force (F_D) arises from the rate of momentum exchange between the charge carriers and the ion. This force is in the direction of electron flow for n type conductors and in the direction of hole flow for p type conductors.

It is believed that because of shielding electrons, the force on the ion due to the electric field is small compared with the force due to the effects of "electron wind drag." Thus, contrary to the random diffusion which takes place in an unpowered conductor where any ion which is a near neighbor to a vacancy has an equal probability of exchanging positions with that vacancy, in a powered n type conductor that ion which is upstream in terms of electron flow has the greatest probability of occupying the vacancy position. This directional effect causes ions to migrate or diffuse downstream in terms of electron wind direction and vacancies move

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upstream.

Metal films as deposited in our industry consist of an agglomeration of single crystal grains where the crystal structure of each grain is oriented in a different direction than any of its adjacent neighbors. (Figure 4). Those lattice ions at the edge of a grain boundary have fewer near neighbor ions than ions within the lattice and as a result the potential wells holding the grain-boundary ions to the lattice are substantially shallower. The measured value for the activation energy of aluminum for grain boundary diffusion has been reported to be 0.55 eV[2]. Thus grain boundaries provide easy paths for self diffusion and electromigration as compared to diffusion and electromigration through the lattice. The surface of the metal can also be considered to be similar to a grain boundary providing an easy path for diffusion. In thin films where the surface-to-volume ratio can be large, surface diffusion may be a significant factor in the total diffusion process.

The net force for an n type conductor is written as:

$$F = F_E - F_P \qquad (1)$$

The exact theoretical understanding of the frictional force due to the electron "wind," F_P, has been the subject of many studies and has yet to be resolved. The resulting net force in the above equation is usually written as:

$$F = Z^* eE \qquad (2)$$

where Z^*e is an effective charge assigned to the migration ion.

Experimentally the force is not directly measurable but what may be observed is the ion flux or the effects of the ion flux produced by that force. Measurements of the ion flux are difficult to perform however the effects of the divergence of the ion flux in thin films experiments are observable as hillock or void formation. It is the growth of voids at regions of divergence of the ion flux that result in the common electromigration failure mode of an open circuit in a thin film conductor.

The ion flux can be expressed as:

$$J_{ion} = N \bar{v} \qquad (3)$$

where N is the density of atoms and $\bar{v}$ is the ion drift velocity. The drift velocity is related to the force by the Nernst-Einstein equation:

$$\bar{v} = MF \qquad (4)$$

where M = mobility = D/fkT

- D = self diffusion coefficient = $D_o e^{-Q/kT}$
- f = a correlation factor depending on the lattice type
- k = Boltzmann's constant

Utilizing the relationship $E = \rho J$ where ρ is the volume resistivity and combining the last three equations results in the relationship:

$$J_{ion} = \frac{N D_o e^{-Q/kT}}{fk} \; qZ^* \rho J \qquad (5)$$

which predicts that the ion flux is a function of J to the first power as is observed in bulk metal[3,4,5].

In the semiconductor industry to determine the electromigration ability of a particular metallization the median time to failure (MTF) by an electrical open is usually measured. This is the time it takes for 50 percent of a sample of conductors stressed identically to fail. The open in the film is caused by an accumulation of vacancies by a positive divergence in the ion flux. The main factors producing the divergence of flux are still under study but appear to be temperature gradients along the metal stripe, structural variations such as grain size, grain orientation, etc. and compositional variations.

Chhabra and Ainsley[6] have shown that temperature variations resulting from Joule heating of the metal stripe produce a divergence in ion flux which is proportional to the current density cubed. Also, in

$$\text{DIV } J_{ion} \propto \frac{J^3}{T^3} D_o e^{-Q/kT} \qquad (6)$$

order to obtain the divergence of ion flux due to structural variations they assumed that sites exist where all of the vacancies are trapped and arrived at a relationship where the divergence of J_{ion} was proportional to the current density,

$$\text{DIV } J_{ion} \propto \frac{J}{T} D_o e^{-Q/kT}. \qquad (7)$$

There is no obvious relationship between the divergence of ion flux and MTF. Black[7,8] has shown that MTF is proportional to the cross sectional area of the film and as a first approximation it can be assumed inversely proportional to the divergence of the ion flux.

$$\text{MTF} \propto \frac{A}{\text{DIV } J_{ion}} \qquad (8)$$

Assuming (as most investigators do) that there are no temperature gradients and the divergence of the ion flux is caused by structural variations in the conducting stripe the last two equations result in:

$$\text{MTF} = \frac{K A T}{J D_o e^{-Q/kT}} \qquad (9)$$

where K is a constant of proportionality.

Invoking temperature gradients as the major cause of ion flux divergence and employing equations 6 and 8 results in the relationship:

$$\text{MTF} = \frac{K^* A T}{J^3 D_o e^{-Q/kT}} \qquad (10)$$

where K^* is a constant of proportionality.

Equation 9 predicts MTF to be an inverse function of current density while equation 10 predicts MTF to be an inverse function of current density cubed. The experimental thin film data of Black[7,8] and more recently that of d'Heurle[9] where current densities in the range 10^5 - 10^6 A/cm^2 were employed indicate the power of J to be between 2 and 3. This agrees well with the results of theoretical studies by Venables and Lye[10] who have considered temperature gradients along with the effects of voiding and arrived at the power of J to be a function of the current density. They found that at low current densities (10^3-10^5 A/cm^2) used in experiments for powering bulk metal the power of J = 1. At current densities of 10^5 - 10^6 A/cm^2 where well heat sunk films can be powered without melting the exponent of J lies between 1 and 3.

That the effects of temperature gradients should

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be considered is emphasized when one computes the power density dissipated in aluminum by Joule heating at high current densities. The power density in watts per cm^3 can be expressed as:

$$\frac{\text{Watts}}{\text{cm}^3} = \rho \; J^2 \qquad (11)$$

For Al at 100^oC, $\rho = 3.5 \times 10^{-6}$ ohm centimeters and at $J = 10^6$ A/cm^2 the power density calculates to be:

$$\begin{aligned}\frac{\text{Watts}}{\text{cm}^3} &= \rho \, J^2 \\ &= 3.5 \times 10^{-6} \times (10^6)^2 \qquad (12) \\ &= 3.5 \times 10^6\end{aligned}$$

This level of power density can be sustained in Al only by well heat sunk thin films.

It is extremely difficult to experimentally determine the exponent of J. Experimental data plotted as an Arrhenius plot using either 1 or 3 as exponents of J (equations 9 or 10) both yield straight lines with about the same activation energies. Such data taken by Black(7,8) and plotted as an Arrhenius relationship using 2 as the exponent of J is presented in Figure 5. This shows the effects grain boundary and surface diffusion paths have on the lifetime of aluminum films. Conductors made of small grained aluminum (relative to the conductor line width) containing both a high density of grain boundary paths and a large surface for the easy electromigration of aluminum ions exhibit an activation energy for electromigration of 0.48 eV and a relatively short MTF at lower temperatures. (On this plot lifetime increases as the ordinant value decreases). Films formed of large grained crystals (relative to the conductor linewidth) provide easy electromigration paths mainly at the surface and exhibit moderate lifetimes at the lower temperatures and an electromigration activation energy of 0.84 electron volts. Here diffusion down grain boundaries has been minimized. Conductors manufactured with large grain aluminum that have been glassed by chemical vapor deposition techniques using silane to reduce both grain boundary and surface diffusion permit electromigration to take place mainly by lattice diffusion and exhibit the greatest life at the lower temperatures. The activation energy of these films was determined to be 1.2 eV and approaches that of bulk aluminum of 1.48 eV.

Figure 5 shows that the three aluminum Arrhenius plots converge as temperature increases indicating that the structure of the Al films has little effect on lifetime at high temperatures. This is because the diffusion through the crystal lattice at the elevated temperatures becomes so great that it dominates any effects due to grain boundary or surface diffusion.

Figure 5 also contains an Arrhenius plot (dashed line) of an Al-2% Cu alloy which has been proposed to improve the MTF(9). Here the data points marked (X) were obtained by Hall(11) and the two points marked (O) were obtained from d'Heurle(9). The activation energy for the alloy is about 0.6 eV and the MTF is about 40 times larger than that exhibited by small grain aluminum films at all temperatures. Its resistance to electromigration is greater than large grained aluminum films above about 70^oC and greater than large grained glassed aluminum films at temperatures above 175^oC. Thus it appears that this alloy is useful to slow down electromigration at high temperatures, however large grained and glassed pure aluminum appears superior at temperatures below about 175^oC. It has been reported that increasing the copper content to 4% further improves the performance of the alloy(9).

Motion Picture of the Effects of Electromigration

A motion picture taken by means of a scanning electron microscope (SEM) shows the effects of electromigration in films stressed at high levels of current density and temperature. Three different sequences of the film are briefly described in the following paragraphs.

Large Grained Al Films at High Temperature

A large grained non-glassed aluminum film conductor deposited on 1 μ thick SiO_2 supported on silicon was stressed at a current density of 1.4×10^6 A/cm^2. Because of poor heat sinking of the device it is estimated that the film temperature in the vacuum ambient of the SEM was about 240^oC. At this temperature the predominant mechanism of electromigration is by diffusion through the crystal lattice. The film showed triangular shaped voids (Figs. 6a and 6b) formed by the condensation of vacancies that move upstream in terms of electron flow. The shape of the angular voids is caused by the void faces lying on the (111) planes in the individual grains. As the voids move across grain boundaries their shape alters when they penetrate the new grain because of the change in direction of the (111) planes. Also as a void crosses a grain boundary, the grain grows back in a shape nearly identical to the shape it possessed before the void traversed it.

This sequence showed the voids migrating several tens of microns in real time. Figures 6a and 6b are sequential in time show the void motion from left to right in a stripe where the electrons flow from left to right. At times the voids consumed greater than 50% of the film cross sectional area however failure did not occur at these sites. The film failed at the negative end of the stripe where due to gradients in temperature and current density the voids clustered to form a near open circuit. This resulted in excessive heating in the narrow conductor causing melting and finally dewetting of the molten metal to form the open circuit.

Large Grained Al Films at Moderate Temperature

The second movie sequence showed electromigration occurring at lower temperatures in large grained non-glassed aluminum films where grain boundary and surface diffusion predominates. This is in the temperature range where most devices operate and depicts the more usual form of electromigration encountered in real parts. With grain boundary and surface diffusion predominating void migration through the grains is not observed. The sequence showed a single grain of aluminum with a grain boundary triple point on each side of the grain. Originally when powered with the electron flow from left to right (Fig. 7) a void was formed on the left side of the grain at the triple point and a hillock was formed on the right side of the grain (also at the triple point). The void formed because at that triple point there were two easy paths around the grain for the transport of mass by electromigration away from the region while there was only one easy path to bring mass (from upstream) to that triple point. The excess generation of vacancies by this process caused the void to grow.

In a like manner a hillock grew at the triple point downstream from the grain. Mass was transported to that triple point by means of the two easy grain boundary paths (around the grain) at a rate greater than mass could be transported away from that triple point by a single grain boundary. The metal ions accumulated in that region to cause a hillock of aluminum.

This sequence also demonstrated the effect of the reversal in direction of electron flow. Figure 8 is a

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view of the same grain as in Fig. 7 but after the current was reversed for a short period of time. This now shows a void growing at the triple point to the right of the grain and the void which previously grew to the left is reduced in size as the excess metal ions accumulate in that region.

Al - 2% Cu Alloy

The electromigration effects in a Al-2% Cu alloy film conductor was the last sequence shown in a film strip taken by means of the SEM. The conductor was deposited on thin thermally grown SiO_2 on silicon which contained an underlying junction. The configuration enabled surface topology studies using secondary electrons and mass density studies using the electron beam induced current mode (EBIC) of the scanning electron microscope. In the EBIC mode electrons which are transmitted through the film and enter the silicon generate electron-hole pairs which are collected at the p-n junctions and used to modulate the grid of the SEM's cathode ray oscilloscope. The strength of this signal depends on the metal film thickness and its mass density. The Al-2% Cu film consists of copper rich precipitates ($CuAl_2$) in an aluminum matrix. Since these regions are denser than the pure aluminum they appear as dark regions. Figure 9 shows an EBIC display of the film as deposited on a 150°C substrate in a vacuum by thermal evaporation of the alloy. Electron microprobe analysis of the film indicated that it had a nominal composition of 2 wt % copper. The dark particles were identified by the electron microprobe to be $CuAl_2$. These consist of large particles (α 2500 Å) mainly on the surface but also in the bulk of the film, and a group of much finer particles less than 700 Å in diameter in the interior of the film distributed along grain boundaries and at triple points.

When powered in the SEM at about 300°C initially the larger surface particles coarsened and those larger particles in the interior of the film disappeared. Due to electromigration those surface large particles at the positive end grew the largest while those at the negative eventually disappeared. Figure 10 shows the negative end of a conductor stripe after it has been depleted of surface precipitates. The coarsened surface particles to the left of this figure have grown to about 1-2 microns in diameter with a height of about one micron and extend along the stripe to the positive end.

Aluminum ions also migrated from the negative end of the stripe causing thinning of the stripe. Since no general voiding was evident as is experienced with pure aluminum films it appears that major electromigration path was over the surface of the film. Apparently the small copper rich participates in the film interior are stationary and prevent grain boundary diffusion while aluminum electromigration can take place over the surface after the surface has been depleted of the participates.

Voids in the film at the negative terminal as shown in Fig. 10 initiate at the edges where presumably thermal gradients are the greatest. Later voids also grow in the middle of the film as the film thins. Eventually the voids extend across the entire structure at the negative end causing failure and an open electrical circuit.

Summary

Electromigration can be considered to result from the normally random self diffusion of aluminum being altered to a directional process by frictional forces caused by the charge carrier "wind." The diffusion which occurs preferentially in the direction of charge carrier flow results in mass being transported in that direction. Since in close spaced crystalline structures (like aluminum) diffusion takes place by an ion exchange with a near neighbor vacancy, vacancies electromigrate upstream (in terms of charge carrier flow). Divergence in ion flux causes vacancies to condense to form voids (which eventually may grow to form an open circuit) and ions pile up to cause hillock and whisker growth.

The causes of ion flux divergence are poorly understood but have been attributed to temperature gradients, structural gradients and compositional gradients. It is difficult to relate MTF of a given conductor to the divergence of ion flux, however, for thin films powered at 10^5 to 10^6 A/cm^2 the MTF has been found by experiment to be inversely related to the current density raised to the second or third power.

At temperatures below about 225°C the structure of the film plays an important role with films providing easy electromigration paths down grain boundaries and over the surface exhibiting the shortest lifetime. The addition of 2% copper to aluminum appears to enhance the lifetime of small grained aluminum by about 40 times at all temperatures. The alloy also exhibits longer lifetime at temperatures greater than about 175°C than does large grained and glassed pure aluminum film. The latter, however, appears preferable at the lower temperatures.

The importance of good heat sinking of the film conductors is stressed since enormous gradients in temperature may occur when the power density due to Joule heating easily can approach or exceed the 10^6 watts/cm^3 level.

Acknowledgements

In preparing this survey paper I have relied heavily upon the work and council of my co-workers. For the preparation of the SEM motion pictures showing the effects of electromigration I am pleased to recognize the efforts of Mr. Anthony Gonzales, Dr. Elliott Philofsky and Dr. Edward Hall. I am further indebted to Dr. Edward Hall for his work on the electromigration of aluminum-copper alloy and for his valuable general council on electromigration.

Footnotes

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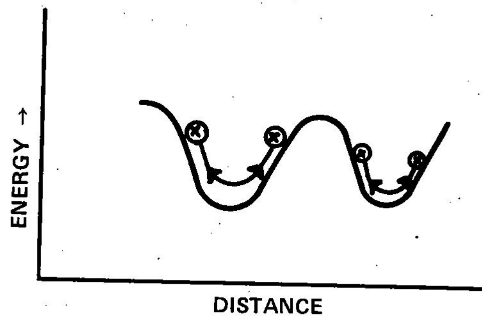

Figure 1. Metal ions oscillating in potential wells.

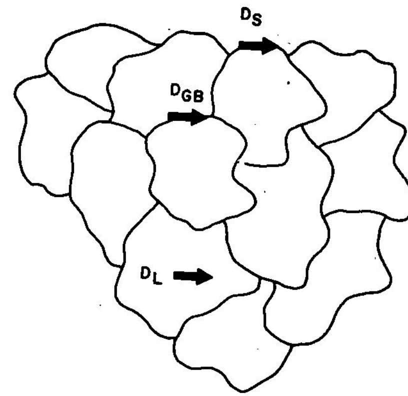

Figure 4. Lattice, grain boundary and surface diffusion.

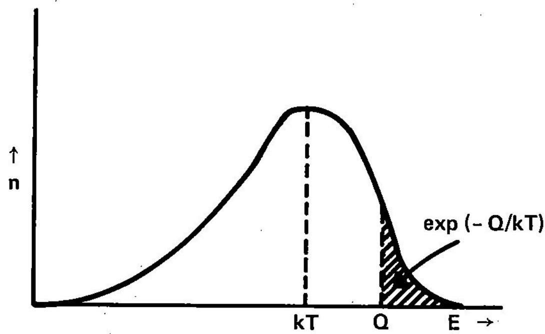

Figure 2. Distribution of thermal energy.

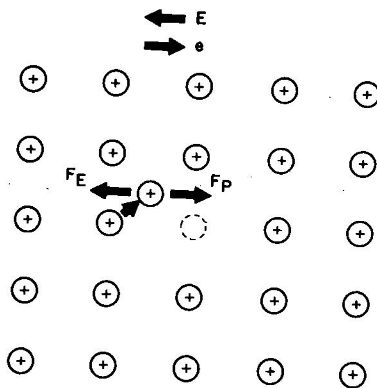

Figure 3. An ion in the process of exchanging position with a near neighbor vacancy.

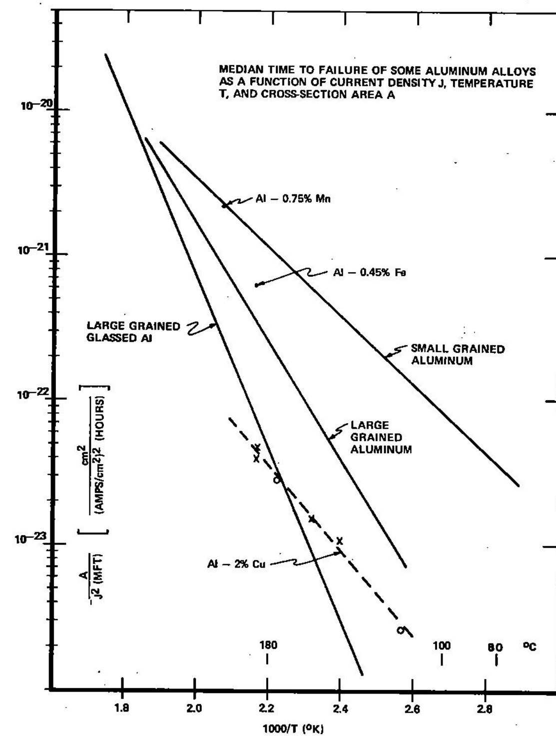

Figure 5. Median time to failure of some aluminum alloys as a function of current density J, temperature T and cross sectional area A.

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Figure 6. Sequential pictures showing void motion in large grain aluminum.

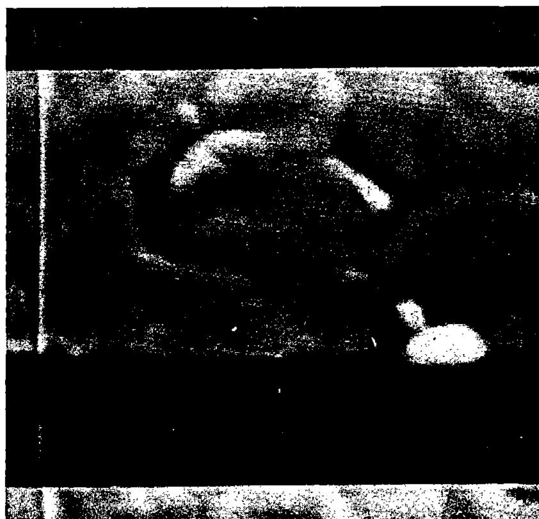

Figure 7. Grain boundary electromigration with electron flow from left to right.

Figure 8. Grain boundary electromigration with electron flow from right to left.

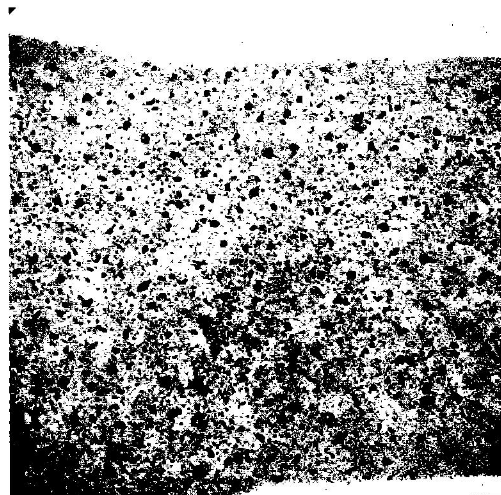

Figure 9. EBIC display of Al-2% Cu film as deposited.

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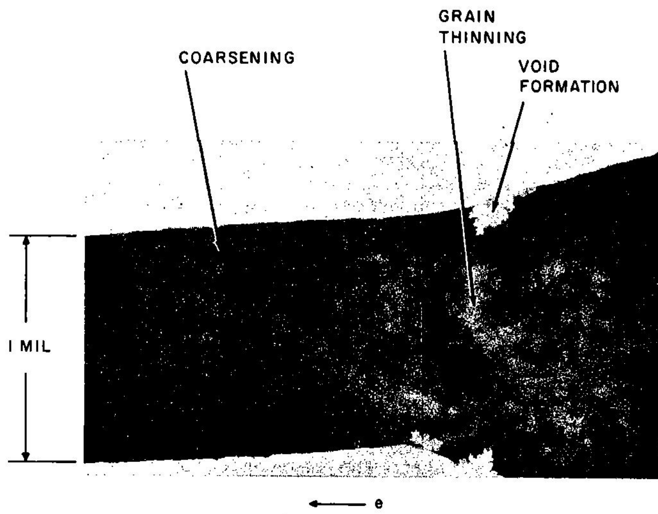

Figure 10. EBIC display of negative end of Al-2% Cu after electromigration.

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