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Experimental study of electromigration in bicrystal aluminum lines

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We report a new experimental technique for the study of electromigration in Al lines containing controlled, single, identical grain boundaries with boundary planes perpendicular to the plane of the substrates. We show that failure times of these lines are lognormally distributed; that the median time to failure depends more strongly on the boundary orientations than the types of grain boundaries; that the deviation in the time to failure has a large component not dependent on microstructure; and that both interfacial diffusion and grain boundary diffusion appear to contribute to failure in bicrystal lines, and likely in bamboo and near-bamboo lines.

It has been established that the reliability of interconnects depends strongly on their microstructures and dimensions.[1] For example, Cho and Thompson[2] have characterized times to electromigration-induced failure in lines with a wide variety of microstructures, and found that both the median time to failure (MTTF) and the lognormal standard deviation in the time to failure (DTTF) depend on the grain size relative to the line dimensions. They showed that the trends for MTTF and DTTF can be explained qualitatively using a simple "failure unit" model in which the number of failure sites or units is assumed to scale with the number of grains, and therefore the number of grain boundaries, and an interconnect is assumed to be composed of a series of parallel units. The probability of failure of a line, $G(t)$, is related to the probability of failure of individual "failure units," $F(t)$, by

$$G(t)=1-[1-F(t)^{w/d}]^{l/d}, \tag{1}$$

where w, l, and d are the line width, line length, and grain size, respectively, and $G(t)$ and $F(t)$ are the cumulative distribution functions (cdfs) for lines and units, respectively. As device densities are increased, line dimensions have decreased to micron and submicron levels, making individual failure units, e.g., grain boundaries, more significant in contributing the line failures. Our goal is to provide an improved understanding of the statistics and mechanisms of interconnect failure by concentrating on the failure of individual units.

Figure 1 illustrates the technique we developed to test populations of Al lines, each with a single, identical grain boundary, and with controlled orientations and locations. We start by cutting two NaCl single crystals with the desired orientations and geometry. The desired planes are polished and the two crystals are welded together using AgCl. The resulting bicrystal is polished in the same manner (see Hsieh[3] for details). We next grow an epitaxial, bicrystal Al film on the NaCl bicrystal substrates. To establish the best deposition conditions, we have tried many different deposition techniques, vacuum conditions, deposition rates, and substrate temperatures. We found that the optimum parameters are the use of thermal evaporation at a rate of about 500 Å/s, at a substrate temperature of 350 °C, and with a background pressure of 2×10^{-6} Torr. The films were then floated off the NaCl substrates, rinsed well in deionized water, and carefully transferred to an oxidized Si wafer. A light pressure was applied to smooth out the films, and a weight was applied during drying. Photolithography and ion milling were used to pattern the bicrystalline films with a modified version of a previously reported test pattern[4] [see Fig. 1(d)], which allows simultaneous wafer-level testing of multiple parallel lines. In this modified version, the test lines are alternated with "reference" lines not connected to the contact pads. The test pattern mask also contains reference marks to allow patterning with the position of the grain boundary at various angles to the direction of the current flow. In Fig. 1(d), the boundary is positioned normal to the current direction. Prior to testing, the wafers were annealed in air at 300 °C for two weeks to bond the Al films to the substrates through the reduction of SiO_2 to form Al_2O_3 at the inter-

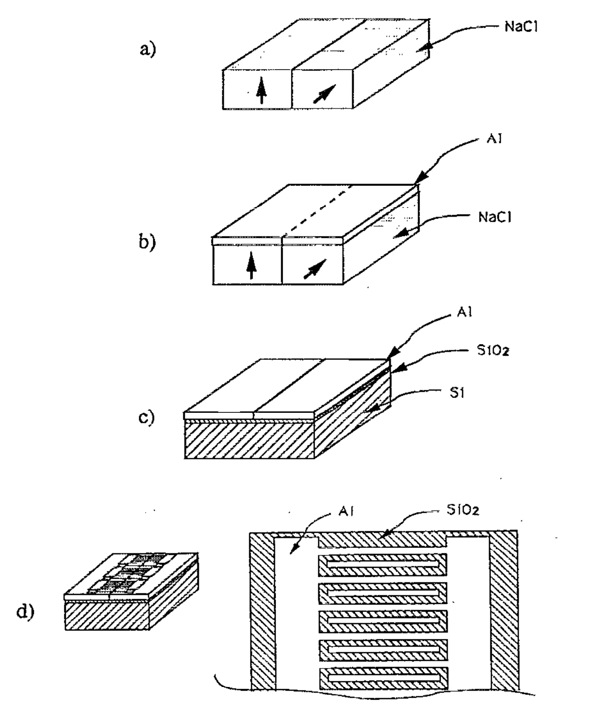

FIG. 1. The fabrication process of bicrystal test patterns. (a) NaCl bicrystal substrate made from two NaCl single crystals; (b) Al bicrystal thin film epitaxially deposited on the NaCl substrate; (c) Al film transferred to an oxidized Si wafer; and (d) patterning.

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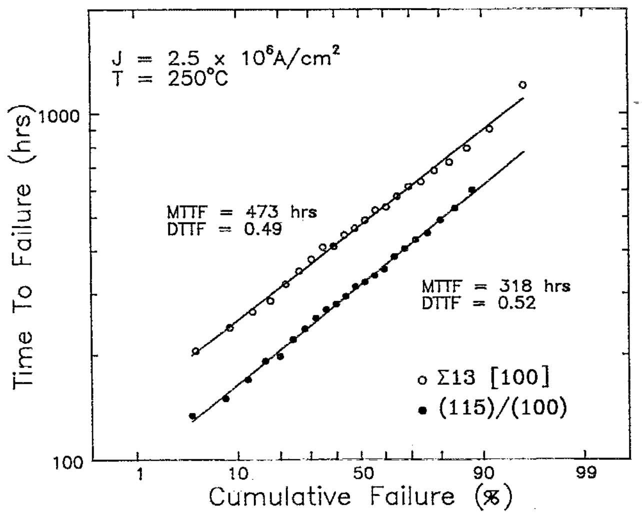

FIG. 2. Failure distributions of two types of bicrystal lines containing two different types of grain boundaries: A symmetric tilt boundary Σ13[100] and a general boundary (100)/(115).

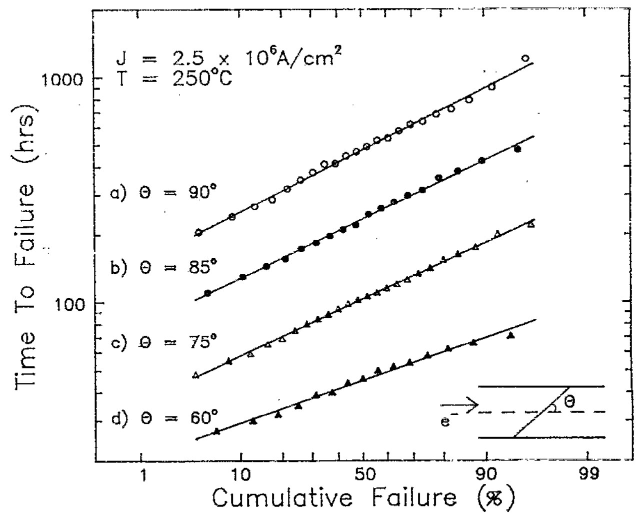

FIG. 3. Failure distributions of Σ13[100] bicrystal lines as a function of φ the angle between the current direction and the grain boundary plane.

face. This process leads to growth of a thin Al_2O_3 layer on the free surfaces of the lines. The Al film thickness was about 5000 Å, and the lines were 1 mm long and 2 μm wide. Lines were tested at a constant voltage, at 250 °C, and at a current density of 2.5×10^6 A/cm^2.

To study the effect of the type of grain boundary on electromigration, we selected two types of grain boundaries: $a\Sigma=13[100]$ symmetric tilt boundary ($\Sigma\equiv$the reciprocal of the fraction of atoms in coincidence)[5] and a (115)/(100) boundary. The Σ13[100] boundary was made by welding together 2 cubic crystals misoriented by a rotation of 22.62° around a common ⟨100⟩ axis, resulting in a {510} boundary plane. This boundary was chosen as a low coincidence site density boundary which is not faceted and is known to retain ordered structures at temperatures as high as $0.96T_m$.[3] The (115)/(100) boundary was produced by welding the sides of two rectangular NaCl single crystals together. The orientation between the two crystals was (115)//(001) and [230]//[100], and the boundary was formed between the (321) plane of the (115) crystal and (010) plane of the (100) crystal. This boundary is considered a general boundary.

Because of the many processing steps required to produce the test pattern it was deemed necessary to perform checks for reproducibility by producing and testing several patterns of each type of boundary. We tested eight (115)/(100) and ten Σ13 [100] test structures each containing 22 lines. We obtained MTTFs of 300±30 h and 480±40 h and DTTFs of 0.48±0.05 and 0.52±0.06 for the (115)/(100) and Σ13[100] boundaries, respectively.

The failure times of both types of boundary are well fit by a lognormal distribution as shown in Fig. 2. This appears to agree with the lognormal assumption of Cho and Thompson's failure unit model.[2] It is important to note that since $F(t)$ is the cdf for a lognormal (LN) distribution, $G(\bar{t})$ for bamboo lines is expected to be the cdf for a multiple lognormal (MLN) distribution. While experimental results for small populations of lines might fit both LN and MLN distributions, the use of the proper distribution for predicting the reliability of large populations of lines is critical.[6]

To check the validity of our results, we compared the MTTFs obtained for the bicrystal lines to the MTTFs reported for various types of microstructures ranging from polycrystals,[7] bamboo structures,[7,8] and single crystals.[9,10] To provide a direct comparison between these findings and our own, all the MTTFs are normalized to our testing conditions assuming an activation energy of 0.5 eV for grain boundary diffusion (polycrystals), 1.4 eV for lattice diffusion (bamboo and single crystals), and a current density exponent of 2. The MTTFs for Al bicrystal lines obtained in this study (473 h and 318 h) appear to be of the appropriate order of magnitude; smaller than those of single crystal [4500 h (Ref. 9) and >222 h (Ref. 10)], but higher than those of a bamboo structure [165 h (Ref. 7) and 57 h (Ref. 8)], and orders of magnitude higher than those of polycrystalline materials [0.2 h and 1.7 h (Ref. 7)]. The long lifetimes of the bicrystal lines and the good reproducibility of the results, seem to confirm their integrity. These results also demonstrate that this sample preparation technique is a viable means of producing single crystal as well as bicrystal interconnects. The sequence of line failures appeared to be random with respect to their position in the multiline pattern. This suggests that the temperatures of the lines were the same.

The failure distributions as a function of φ, the angle between the current direction and the grain boundary plane, is shown in Fig. 3. While the DTTFs remain fairly constant, the MTTFs vary strongly with φ. If grain boundary diffusion is the only failure mechanism, we would *not* expect any failures since the diffusion path (i.e., the line width $x\sin\varphi$) is less than three microns, which is much shorter than the Blech length.[11] Also, the appearance and location of the failure sites indicate that the failure mechanism is likely to involve an accelerated grain boundary

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grooving induced by electromigration. This mechanism which involves surface diffusion, was proposed by Ohring to explain the film thinning and damage observed in stressed films.[12] *Our results therefore suggest that diffusion at the Al/Al_2O_3 interface plays an important role in failure of these lines.* However, further studies, such as *in situ* TEM electromigration experiments, as well as measurements of the temperature and current density dependence, will provide more conclusive evidence of the failure mechanism.

The reproducibility of our results shows that the measured difference in the MTTFs of the two types of boundaries is real. Diffusion along the higher energy, asymmetric (115)/(100) grain boundary is expected to be faster than along the lower energy, symmetric $\Sigma 13$ [100] boundary.[13,14] If we assume that electromigration-induced diffusion along the grain boundaries does play a role, even for $\varphi = 90°$, we might expect a correlation between MTTF and the grain boundary diffusivity such as illustrated in Fig. 2. An alternative explanation for the difference in the electromigration resistance, regardless of the failure mechanisms, would be that grain boundaries are considered to be sources and sinks of vacancies, and that the source/sink efficiency tends to be lower in certain special low Σ, low energy boundaries, than in more general, high-energy boundaries.[15,16]

If the primary diffusion paths are along the Al/Al_2O_3 interfaces, we would still expect the line intercept of the grain boundary and the interface to be the site of a divergence of the point defect flux. When φ is 90°, we would expect little or no diffusion along the grain boundary. However, as φ is reduced, more diffusion along the grain boundary would be expected leading to a greater flux divergence, and a shorter time to failure. As illustrated in Fig. 3, this is what is observed. Moreover, the view that the grain boundary functions only to divert transport along the interface would explain why $\varphi = 90°$ does not appear to be a singularity, in that the MTTF at $\varphi = 90°$, and the 90° value extrapolated from the results at other angles, appears to be finite. We note in passing that the data are well fit by the function:

$$\text{MTTF} \alpha [1 + \beta \cos \varphi]^2$$

where β has the value 4.9, and might be interpreted as related to the ratio of the grain boundary diffusivity to the differences in the interface diffusivities.[17]

The DTTFs are finite and do not appear to vary with the type of grain boundary. If we assume that DTTF is the result of microstructural variations alone, the DTTF of identical failure units should be zero. The variations in lifetimes may have resulted from both intrinsic and extrinsic causes. Intrinsic variations are likely to be atomistic such as surface roughness, dislocation densities, boundary structures, etc. External causes result from processing-related variations in film thickness, line widths, adhesion, etc. Although the DTTFs of 0.5 for the bicrystal lines tested here are comparable to those of polycrystalline lines, they are smaller than the values of > 0.7 reported for bamboo structures.[7,8] The larger DTTF in bamboo lines is likely the result of microstructural variations such as the presence of triple junctions in near bamboo lines, or variations in the orientation of the bamboo grain boundaries with respect to the current direction.

In summary, we have developed a new experimental technique which allows statistical analyses of electromigration in large populations of lines with identical single grain boundaries of chosen types, locations, and orientations. Our preliminary results show that the technique is quite reliable, and suggest that (1) the failure times for lines with single identical grain boundaries are lognormally distributed: (2) The MTTFs are only weakly dependent on the type of boundary (for bamboo structures); (3) the DTTFs are finite in lines with "identical" microstructures, and (4) Al/Al_2O_3 interfacial diffusion contributes to failure of bicrystal lines (and likely of true and near-true bamboo lines as well). This result suggests that interfacial diffusivities are comparable to grain boundary diffusivities in these materials. This interpretation indicates that suppression of interfacial diffusion, and the associated grain boundary grooving, should lead to improved reliability of bamboo lines.

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