Defect behavior in aluminum interconnect lines deformed thermomechanically by cyclic joule heating

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Abstract

Al–1wt.% Si lines were deformed thermomechanically by cyclic joule heating induced by applying an AC current. Scanning electron microscopy revealed arrays of wavelike surface intrusions/extrusions aligned along low-index crystallographic directions after a few thousand thermal cycles. Transmission electron microscopy observations of cross-sections of selected regions shows that in grains that developed intrusions/extrusions, dislocations nucleated at the film–substrate interface, glided to the surface, and escaped. The densities of dislocations and prismatic loops observed here are similar to those observed in mechanical fatigue experiments on bulk aluminum.

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1. Introduction

Interest in the reliability of thin-film metal lines on silicon substrates arises because narrow lines of physical vapor deposition (PVD) aluminum and electrodeposited copper are widely used to form interconnect structures in ultra large scale integration (ULSI) microchips. While the lines studied in this work are not buried in dielectric like most interconnects, the test techniques and failure mechanisms explored here may provide useful information for designers of future interconnect structures.

Scanning electron microscopy (SEM) showed that arrays of wavelike surface features were generated when passing low-frequency, high-density AC through long narrow lines of thin-film aluminum [1–3]. However, in those works the specific mechanism by which the surface features were formed was not discussed. It should be noted that similar wavelike surface features have been observed in several studies of copper films subjected to AC current and attributed to thermomechanical or AC fatigue [4–6]. Here also there were no discussions detailing the mechanism by which the surface features were formed.

Surface features that result from cyclic mechanical strain are well documented in research on the mechanics of fatigue deformation in both thin films and bulk specimens. Almost all of the studies have been done on copper [7,8]. Schwaiger et al. [9] studied mechanical fatigue of polycrystalline copper films of various thicknesses on polyimide substrates. They observed extrusions on the film surfaces and voids at the film–substrate interface, and described transmission electron microscopy (TEM) investigations that showed that no long-range dislocation structures developed during fatigue. Probably the best classic example of the extrusion/intrusion surface structure resulting from fatigue in a bulk material was given by Basinski and Basinski [10]. Cord and tweed surface structures were described by Videm and Ryum in cyclically deformed [001] aluminum single crystals [11].

Some previous reports of TEM observations on thermally cycled aluminum thin films are available. Legros et al. [12,13] reported TEM observations of dislocation
behavior in passivated aluminum films strained by thermal cycling between room temperature and 450 °C. They observed a decrease in the dislocation density and an increase in the grain size with the number of cycles. A convergent-beam electron diffraction (CBED) study of strains in cross-section samples of Al film cycled approximately 10 times between 150 and 250 °C showed large variations in the strains generated both within grains as well as from grain to grain [14]. TEM studies of the typical dislocation structures of tangles and cell walls that result from uniaxial fatigue of bulk polycrystalline aluminum have also been described in the literature [15,16]. A combined TEM/focused ion beam (FIB) study of fatigued thin copper films [17] reported that when the film thickness was less than 1 μm, with correspondingly small grains, tangled dislocation structures were replaced by individual dislocations.

A combined SEM and EBSD analysis of grain growth and rotation under AC fatigue as used here was reported by Keller et al. [18]. The grains that grew and rotated were the same ones that showed the most pronounced surface intrusions/extrusions.

In this paper we describe what we believe to be the first detailed analysis of dislocations and vacancies resulting from AC fatigue of thin aluminum lines. We interpret the SEM and TEM observations to establish the mechanism of the deformation and to relate it to known effects in mechanical fatigue tests of bulk materials.

2. Experimental

The samples were patterns developed originally for electromigration studies. The aluminum films were fabricated by PVD of Al–1wt.% Si onto oxidized silicon wafers. The line patterns plus test pads were fabricated in a photolithographic process. The dimensions of the lines were 3.3 μm wide by 800 μm long and 450 nm thick (see Fig. 1).

Application of the AC testing technique to interconnect lines has been discussed in detail [3,4,19]. Here we used the same experimental approach. The four test pads associated with each line, defined in Fig. 1, were used for electrical contacts. AC was applied at 100 Hz with an amplitude of 220 mA, resulting in a current density of 14.8 MA cm⁻². DC resistance measurements on similar lines indicated that the maximum temperature range was about 220 °C. The AC testing was done with the chip at room temperature (20 °C), suggesting that the maximum temperature in the line reached approximately 240 °C. Because the coefficients of thermal expansion (CTE) of aluminum and silicon are quite different, with \( \alpha_{\text{Al}} = 2.31 \times 10^{-5} \text{K}^{-1} \) and \( \alpha_{\text{Si}} = 2.6 \times 10^{-6} \text{K}^{-1} \), this temperature change, \( \Delta T \), imposes a significant biaxial strain, \( \Delta \varepsilon = \Delta T \cdot \Delta \alpha \), of approximately 0.3% on the aluminum line. The data reported in this paper were obtained from a sample that was cycled for 40 s, resulting in \( 8 \times 10^3 \) temperature cycles. Under these testing conditions, the lines typically exhibit a lifetime (to open circuit) of approximately \( 1.2 \times 10^5 \) cycles.

After \( 8 \times 10^3 \) cycles, the line exhibited some regions with surface extrusions/intrusions as well as regions with no obvious surface damage. A cross-section including both intrusions/extrusions and undeformed regions was prepared for TEM by focused-ion-beam (FIB) milling. TEM was done at 200 kV using a LaB₆ gun and a double-tilt goniometer sample holder. Images were collected with a 1 Mpixel CCD camera.

Dislocation densities were obtained from a number of micrographs by digitally measuring the total length of dislocation lines visible and calculating the length per unit volume. The dislocation densities given are a lower bound since we did not do a complete diffraction vector analysis of every region. Prismatic dislocation loops were also observed; their densities were obtained by digitally defining the visible loops in a micrograph and obtaining the mean diameter and total number of loops in each micrograph. Again, the densities given are a lower bound. Artifacts from the FIB milling were handled by utilizing the difference between tested and untested lines, both prepared by FIB milling.

![Fig. 1. Typical patterned aluminum sample used in the AC tests. The aluminum line is 800 μm long by 3.3 μm wide and 450 nm thick. Current and voltage contact pads are labeled C and V, respectively. The substrate is oxidized silicon/silicon.](image-url)
3. Results

The SEM and the companion EBSD inverse pole figure images of a plan section including both intrusions/extrusions and undeformed regions before FIB milling are shown in Fig. 2 with the FIB section outlined. The EBSD data (Fig. 2b) show that the region with the intrusions/extrusions is a single grain. The orientation matrix for this grain was determined by EBSD to be

\[
G = \begin{bmatrix}
0.6958 & 0.0382 & 0.7173 \\
0.5648 & 0.6460 & -0.5135 \\
-0.4437 & 0.7624 & 0.4710 \\
\end{bmatrix}
\]  

(1)

where the column \([-0.0382, 0.6460, 0.7624]\) that can be reduced to \([-11619]\) corresponds to the crystallographic direction along the line, which is 5.4° from [011]. This EBSD orientation was confirmed with TEM by selected area diffraction from the same region.

Fig. 3 is a bright-field TEM image of a grain that shows no surface intrusions/extrusions in either plan view SEM or cross-section TEM images. The image shows dislocations most likely of edge type with \(b = \frac{1}{2}[101]\) on the \((111)\) slip plane. The visible dislocation density in this micrograph is \(7.9 \times 10^{13} \text{ m}^{-2}\). Other regions examined showed visible dislocation densities that ranged from \(5.4 \times 10^{13} \text{ m}^{-2}\) to \(8.4 \times 10^{13} \text{ m}^{-2}\). Many of the dislocations exhibit bowing that corresponds to a residual stress in the films. The mean value for this stress was about 25 MPa, which was calculated from measurements of the radius of curvature of bowed dislocations using the expression \(\sigma = \frac{Gb}{2R}\), where \(\sigma\) is the residual stress on a bowed dislocation, \(G = 26 \text{ GPa}\) is the shear modulus for Al, \(b = 0.286 \text{ nm}\) is the Burgers vector, and \(R\) is the radius of curvature for the bowed dislocations (nm), which had a mean value of 153 nm for 25 measurements.

Fig. 4 is a weak-beam dark-field (WBDF) image with \(g = [022]\) from a segment of the grain that showed the surface protrusions. The thickness of the TEM section was determined to be approximately 140 nm by use of the CBED technique described in [20,21] and the simulation software given by De Graef [22]. An aluminum oxide film \(\sim 15 \text{ nm}\) thick was found on the surface of the tested lines.

The dislocation density here is very high, \(8.4 \times 10^{13} \text{ m}^{-2}\). However, the dislocations are not distributed as uniformly as those in Fig. 3, but are concentrated at the aluminum/silicon oxide interface and bowed away from the interface, suggesting that they could have been nucleated there.
the most part the dislocations in Fig. 4 also appear to be edge dislocations. The dislocation density in the untested sample was very low, $2.3 \times 10^{12} \text{ m}^{-2}$; this value was determined using the total length of visible dislocation lines.

An unexpected feature seen in all the micrographs from this sample is the very high density of dislocation loops. Both the untested and the tested lines had dislocation loops, but there were clear differences between the two cases. In Fig. 5, which is a micrograph of the typical structure observed in an untested line prepared by FIB, a high density (approximately $1.1 \times 10^{21} \text{ m}^{-3}$) of small dislocation loops can be seen. Since it is highly unlikely that a high density of loops would occur in an untested line, we conclude that the small loops observed in all of these samples were the result of surface damage created by the high-energy (30 keV) Ga$^+$ ions used in the FIB sample preparation. The mean diameter of 119 loops measured in the figure is $11 \pm 4 \text{ nm}$ with approximately 88% of the loops having diameters less than the mean value. A few large loops, having diameters much greater than 18 nm, can be seen near a grain boundary. Since there are so few loops having diameters greater than 18 nm in the untested sample, we assume that dense concentrations of loops with diameters greater than 18 nm in the tested sample were created as the result of the AC testing. For example, a relatively high concentration of larger loops can be seen in Fig. 6, which is a high-magnification BF montage from a region in the tested sample that had extrusions and intrusions at the surface. The density of the large loops in such regions varies slightly, but averages about $2 \times 10^{20} \text{ m}^{-3}$ as measured from five different areas that showed surface extrusions taken along the length of the line. The contrast mechanism, which explains the characteristic appearance of the loops and allows unambiguous identification, is described in Ref. [22]. From the TEM contrast it appears that the loops are similar to the vacancy loops previously observed in quenched and...

Fig. 4. WBDF image of a segment containing extrusions and intrusions. The line prior to testing was 450 nm thick. Most of the dislocations are in the vicinity of the film/substrate interface and generally appear to be coming from that interface and are probably edge dislocations. Note the absence of dislocations near the surface of the extrusion regions.

Fig. 5. Cross-section TEM image of untested line prepared by 30 kV Ga$^+$ FIB. Most of the dots show dislocation loop contrast and are the result of damage by the high-energy Ga$^+$ ions. The mean diameter of the loops is 11 nm and the loop density is approximately $1.1 \times 10^{21} \text{ m}^{-3}$. The dislocation density is $2.3 \times 10^{12} \text{ m}^{-2}$. 
fatigued aluminum [23,15]. Considering the loops as planar arrays of vacancies with an average diameter of 21 nm, the vacancy concentration associated with the large loops in Fig. 6 and in similar structures in the vicinity of the extrusions and intrusions is about $2 \times 10^{-5}$.

4. Discussion

It is clear from the TEM images that the dislocation structures in this AC fatigued film are different from previously reported structures induced by mechanical fatigue in both bulk aluminum [15,16] and thin-film copper [9,17]. In this discussion, we first show that the present observations are consistent with deformation by dislocation motion because: (1) the stresses are sufficient; (2) appropriate slip systems are present; (3) the observed density of prismatic dislocation loops is similar to that observed in fatigued aluminum; and (4) the presence of dislocation loops is consistent with dislocation-based plasticity. Finally, we argue that there are some similarities between the present observations and certain features of persistent slip bands. The overall conclusion is that the surface intrusions/extrusions produced by AC fatigue of thin metal lines result from the generation and motion of dislocations.

4.1. Stresses

It is clear that sufficient stress was present in the sample to generate and move dislocations. An upper limit of the stress required may be taken as 280 MPa, which is the approximate value reported for the room-temperature biaxial yield stress for a 500 nm thick Al film on a Si substrate [24]. It is clear that stresses of this magnitude were produced in the AC fatigue test of the specimen examined here. The mismatch in CTE between the aluminum film and the silicon (oxide) substrate provides that a maximum biaxial stress excursion of $\approx 320$ MPa, using a biaxial modulus for Al of 107.5 GPa, could be created on each thermal cycle of the test. This value is based on the temperature excursion of 220 °C determined by the electrical resistance change and the assumption that the stress is purely elastic. This value is consistent with previous observations in substrate-curvature experiments for an Al film on a Si substrate [24] and high-resolution micro X-ray diffraction results from passivated Al (0.5 wt.% Cu) on Si [25]. Residual stress in the as-received samples was estimated by X-ray diffraction to be near 270 MPa in biaxial tension [3], which is consistent with the values of 230–280 MPa reported in Refs. [24,25]. We propose that, during each heating cycle of the AC test, the residual tensile stress decreases, and that the stress excitations produced by the temperature cycles are sufficient to generate a large number of dislocations, similar to the number seen in pure mechanical fatigue tests.

4.2. Slip systems

The next puzzle posed by the present set of observations is why certain grains deform and produce the surface intrusions/extrusions shown in Fig. 2a after short exposure to AC, while other nearby grains do not. For example, why
did the grain shown in Fig. 4 show extrusions/intrusions while the grain in Fig. 3 did not, even though they are adjacent to each other (grains 14 and 11, respectively, in Fig. 2b). A naïve expectation might be that some grains are oriented favorably for single slip of dislocations, driven by the thermomechanical stress along the line axis, while other grains are less favorably oriented for single slip. But the orientations of the grains examined in the present study of regularly spaced linear surface intrusions/extrusions oriented perpendicular to the line axis were measured unambiguously by EBSD, and were found to be inconsistent with this expectation. The reasoning is that in the deformed grain in Fig. 2 the line direction is near [011] and the surface normal is near [111]; therefore the direction parallel to the extrusions is near [211], which does not include traces from any of the possible (111) slip planes. Consequently, the resolved shear stress for single slip is not the appropriate variable to consider as the effective driving force for dislocation motion for the present case, although single slip may be possible in regions with different crystallographic orientations, such as the one pictured in Fig. 1 in Ref. [1].

Cheng and Laird [26] studied mechanical fatigue in copper crystals with various orientations deformed under uniaxial stress. They found that single slip occurred for some orientations of the stress, while double slip occurred for others, and they developed a criterion for double slip. The Cheng and Laird findings cannot be applied directly to the present case because the stress in the present case was not uniaxial, but rather biaxial, because it arose from differential thermal expansion. Finite element modeling (FEM) calculations for the line-on-substrate system, with the appropriate thickness-to-width ratio, show that the stress in the present case is biaxial over most of the line width, with the stress component across the line equal to about 60% of the stress component along the line. Calculations of the total resolved shear stress (RSS) resulting from this biaxial stress in grains 11 and 14 of Fig. 2 show that the (111)[101] and the (111)[110] slip systems have about equal RSS on them, but that the RSS on the relatively undeformed grain (grain 14 in Fig. 2) is 10–15% less than that in grain 11, which showed clear surface intrusions/extrusions. This is consistent with the findings of Cheng and Laird [26], who proposed that multiple slip will occur only if the ratio of Schmid factors on the considered slip systems is greater than 0.9. It is interesting to note that if only uniaxial stress along the line is considered then the RSS numbers reverse and grain 14 should have shown intrusions/extrusions before grain 11. Thus we conclude that the biaxial stress predicted by the FEM model does apply, and that those grains with the highest biaxial RSS were indeed the grains that initially showed surface intrusions/extrusions.

4.3. Prismatic loops

A prismatic dislocation loop density of about $10^{21}$ m$^{-3}$ was reported for 99.995% Al quenched from 600 °C to iced brine by Hirsch et al. [23]. Considering the average loop diameter to be 20 nm, this density translated to a vacancy concentration of approximately $10^{-4}$, which is approximately the saturation concentration calculated at 600 °C from thermodynamic considerations. The equivalent vacancy concentrations in the present specimens are much lower. On the other hand, Segall and Partridge [15] reported prismatic loop densities of $5 \times 10^{20}$ m$^{-3}$ in thin 99.99% Al sheet specimens fatigued by reverse bending. This value is very close to our measured value for the density of the large loops of $2 \times 10^{20}$ m$^{-3}$ in areas showing surface extrusions. Since Segall and Partridge obtained their data in a mechanical fatigue experiment, the similarity of these results suggests that the AC test conducted here is related to mechanical fatigue testing.

The observation that loops are still present in the specimen after the test allows us to estimate that the maximum temperature was certainly less than 325 °C. This limiting value was determined by extrapolating the data of Silcox and Whelan [27] to determine that dislocation loops in aluminum would disappear at about 325 °C in 0.005 s, the time per cycle at 200 Hz.

This value of the maximum temperature implies that the vacancies are generated by dislocation activity, rather than purely thermal processes, as follows. If we consider that vacancies were generated only by thermal processes and that the maximum temperature reached by the line during the thermal fatigue was less than 325 °C, the vacancy concentration would be $\sim 2.7 \times 10^{-6}$, which is approximately a factor of 100 below the measured concentration. The creation of vacancies by moving dislocations is well established [28–30]. Under the temperature cycles associated with the AC test, the vacancies can diffuse short distances and coalesce to form the loops [31].

Thus we conclude that the bulk of the vacancies are generated by dislocation activity, both as glide debris and as the result of intersections.

4.4. Comparison and contrast with persistent slip bands

Because persistent slip bands (PSB) are characteristic of some fatigue processes in fcc metals, and because PSBs are used to explain the surface intrusions/extrusions observed in those experiments [10,33–35], it is of interest to compare and contrast the present results with PSBs. Initial examination of the TEM micrographs reveals no features characteristic of PSBs. Figs. 3 and 6, which are bright-field images representative of the dislocation structures in regions without and with extrusions/intrusions, respectively, show a distribution of dislocations similar to what might be observed in Stage I deformation of a fcc single crystal. They do not show, however, the matrix channel-vein and/or the PSB ladder-like structure associated with intrusions/extrusions in fatigued metals [34,36]. In Fig. 6, and in the WBDF Fig. 4, from regions showing surface extrusions and intrusions, the visible dislocations are not uniformly distributed but concentrated near the film/substrate interface compared with the more uniform distribution seen in
Fig. 3. Careful measurement shows the dislocation density to be similar in both Figs. 3 and 6 with a value of approximately $1.6 \times 10^{14} \text{m}^{-2}$, which is much higher than would be expected in Stage I deformation. This value is, however, within an order of magnitude of the value of $10^{15} \text{m}^{-2}$ proposed by Grosskreutz and Mughrabi [32] for the dislocation density in PSB walls.

Although the film does not exhibit the typical PSB and channel-vein structure seen in fatigued bulk specimens, the general appearance and size scale of the extrusions and intrusions is similar to that modeled by Brinckmann and Van der Giessen [33], and as such suggests that similar dislocation activity might be involved. An estimate of the number of dislocations required to form a surface extrusion of the height observed, considering a distribution of slip bands like that postulated by Brinckmann [34], shows that about one dislocation must exit the surface for every two fatigue cycles. This is consistent with the value of about one Burgers vector per cycle inferred by Basinski and Basinski [10,35].

Consider the extrusion labeled A in Fig. 7 to be rectangular with height 100 nm and width 200 nm. If we assume this extrusion is the result of escaping edge dislocations with a [110] Burgers vector, $b = 0.286 \text{nm}$, on parallel (111) glide planes that are $70b = 20 \text{nm}$ apart, following Grosskreutz and Mughrabi [32], approximately 3500 dislocations ((100 nm/0.286 nm) $\times$ (200 nm/20 nm) $= 3500$) would have to escape from the surface to account for the 100 nm height of the 200 nm wide extrusion. Considering 8000 fatigue cycles, this reduces to about one dislocation every two fatigue cycles.

We also found that EBSD patterns from grains with surface intrusions/extrusions have a higher image quality factor than grains without, indicating less variable elastic strain. This is due to lower dislocation content, and is consistent with our hypothesis that many dislocations have exited the surface in the extruded regions. This is consistent with the TEM observations of lower dislocation content near the surface of the extrusions as seen in Fig. 6.

The overall picture that emerges is that the surface intrusions/extrusions discussed here are clearly not PSBs since the matrix vein and PSB ladder structures are not present here. Another difference is that the surface intrusions/extrusions observed here occurred after fewer than $10^6$ fatigue cycles, while PSBs typically occur after $10^6$ cycles. On the other hand, this AC fatigue experiment does have certain features in common with PSBs. Specifically, we observe regions where many dislocations escaped the specimen surface, leaving behind intrusions/extrusions, and we also observe adjacent regions with dislocation density equal to, within an order of magnitude, the dislocation density in the walls within PSBs.

5. Summary and conclusions

We have shown that a very high density of dislocations exists in films subjected to AC fatigue. They are generated by stresses that result from the difference in the CTE between the aluminum film and the silicon substrate, most likely at the film substrate interface. The stress system is biaxial, with the major component along the length of the line. The grains that show intrusions/extrusions are oriented such that they have the highest resolved shear stresses in the available double-slip systems, providing the mechanism for the dislocations to glide to and exit from the surface. Along with the dislocations, there is a moderate density of prismatic dislocation loops. Their presence is consistent with the dislocation mechanism and provides an upper limit to the temperature, but does not contribute to the deformation. The TEM observations reported here confirm that the regular wavelike surface features produced by AC fatigue are a result of dislocation motion, rather than any purely thermal process like mass diffusion or local melting.

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