Reliability Challenges in Emerging IC Metallization Technologies

J. R. Lloyd
Jet Propulsion Laboratory
California Institute of Technology
Pasadena CA

Introduction

Submicron metallization has been a mixed blessing. On one hand lithography and registration for very small structures and line widths have been extremely challenging, On the other hand, the reliability of very fine Al alloy lines, assuming they can be made, has been better than anticipated. However, great care must be exercised in taking advantage of this windfall, since the benefits are highly process and material dependent. Nowhere is this more evident in IC metallization. The issues are very different for Al alloy or Cu conductors.

In addition to changing conductors from Al to Cu, we have the introduction low-k materials as interlevel dielectric. Mother Nature has played a trick in that the dielectric constant and most other desirable properties have an inverse relationship. For instance as the dielectric constant goes down (a good thing), so also does the thermal conductivity (a bad thing). Other properties follow suit. This poses significant challenges in designing in reliability and in operational use conditions.

Paradigm Shift in Conductors

Much conventional wisdom had to be discarded when submicron conductors came into use. The major failure mechanism in thin film conductors is caused by a diffusion phenomenon known as electromigration. (1) Thin film conductors are thermally connected to a relatively large silicon chip heat sink. Much higher current densities can be passed through thin film conductor line than can through bulk wires. Whereas a bulk wire fuses due to excessive Joule heating at a current density on the order of 10^4 amp/cm^2, a thin film can withstand more than 10^7 amp/cm^2.

As electrons are conducted through a metal, they collide and interact with lattice defects. The momentum exchange from these collisions produces a driving force that acts on diffusing atoms that is proportional to the current density. At the low current densities used in bulk applications, this is not a problem, but at the higher current densities of thin film applications, the biased diffusion due to this momentum exchange becomes significant.

When thin film devices were first employed over thirty years ago, electromigration was such an important problem that it was feared the industry would be brought to a standstill. (2) One of the big hopes for the semiconductor industry was that solid state transistors would be much more reliable than the fragile heat producing vacuum tubes. Panic spread when the first integrated circuits failed due to a mysterious "cracked stripe" problem in only a few weeks of operation. After much tearing of hair and shedding of tears, electromigration was identified as the culprit.

The reason why it was such a problem is that Al was used as a conductor material. Al is a very forgiving during processing and is an excellent conductor, being the 4th best normal conductor material. However, Al melts at a low temperature, 660C, and this means that diffusion in Al is relatively rapid. Furthermore, the thin film structure is made up of very small metal crystals, or in metallurgist's terms, is extremely fine grained. There is a rule of thumb that the crystal size, or grain size of a metal sheet is on the order of the sheet thickness. In the original thin film devices, the Al conductors were only ~3000A thick and about 10 μm wide. The regions between the crystals, or the grain boundaries, are rapid diffusion pathways since they are relatively disordered compared to the grain interiors. Therefore in these early applications, we had three strikes against us. We had a low melting temperature rapid diffusion conductor, a fine grain size that exacerbated the problem and a very high current density. We struck out.

The solution to the problem came with the discovery that Cu added to the Al slowed grain boundary diffusion enough that the electromigration lifetime was increased to where useful currents could be employed and viable devices could be designed and built. (3) Extensive testing was performed and design rules generated that, when carefully observed, would ensure reliable product.

One important consideration was that processing variables could severely affect the lifetime of Al conductors. Since the major diffusion pathway is the grain boundary, the grain structure was found to be critically important. A larger grain size was obviously preferred as larger grained materials would have fewer grain boundaries, but the grain size distribution was found to be equally if not more important. (4)

For failure to occur due to electromigration, a mass flux divergence is necessary. A non-uniform grain structure will provide regions where the number of grain boundaries changes over a short distance. This will cause an imbalance in the mass flux in these regions leading to depletions (voids) or accumulations (extrusions). Voids caused open circuits and extrusions could cause shorts.

This was the understanding of electromigration reliability. The grain size had to be large to reduce the number of fast diffusion pathways, and the grain size had to be uniform to obviate flux divergences. Two developments in IC technology, however, changed this simple picture. First, the maturation of metal deposition techniques allowed grain sizes larger than the rule of thumb allowed, and the line widths became much smaller.

As the line widths became smaller, the reliability at first suffered. A narrower line, given a typical grain size distribution (typically lognormally distributed with the standard deviation, σ, around 0.5) had a higher probability of containing a structurally induced flux divergence than a wider line. This trend continued as the lines became narrower, but then reversed when the line width became less than about 1.5 times the grain size. For these narrower lines, the reliability suddenly improved dramatically. Film thicknesses of ~ 0.5 μm had become common and well-behaved grain size distributions with medians of more than 2 μm were often achieved. Under these conditions, the lifetimes of 1 μm wide conductors were as much as an order of magnitude longer than those twice as wide. (5,6)

The reason for this windfall was that when the line width is much smaller than the grain size we achieve what we call a "bamboo structure" where all the grain boundaries meet the line edges before they meet another grain boundary. Thus we no longer have a continuous network of grain boundary pathways like we did in wider lines. Thus, electromigration must proceed via other more difficult and slower diffusion mechanisms, such as through the lattice or along interfaces.

Thus, if we can assure a large grain size, we can pass about three times the current density through narrower lines than we can through wider ones. However, to take advantage of this, we must be absolutely sure that the grain size is well behaved and that the grain size does not change from day to day. Periodic measurements of the metallic grain size have become common in the industry to reflect this concern. It must also be kept in mind that not all the conductors in an IC are narrow. Bus lines and clock lines tend to be wider and the reliability will suffer accordingly. This is a cruel trick played by M. Nature in that conductor lines are made wider to accommodate higher currents, yet are inherently less reliable. Line width dependent design rules have been adopted to account for this.

Effects of Stress

The hallmark of the past 5 years of study into electromigration failure has been the increased understanding and the appreciation of the role of mechanical stress. As we now understand it, electromigration failure will occur when the induced stress reaches a critical value. Tensile stresses will form voids or cracks and compressive stress will form extrusions. (7)

The behavior of thin films carrying high current density is determined by the curious way electromigration interacts with mechanical stress. The driving force that stress imposes on mass transport is not the level of stress but the stress gradient. If the stress were uniform, regardless of the magnitude, there would be no stress-assisted diffusion. An anthropomorphic analogy would be that on a hot summer day if all rooms in a house were equally uncomfortable one would not hold a preference for one over the other. If, however, one of the rooms were air conditioned, there would be a definite migration in that direction.

In the presence of flux divergences, such as contacts to the semiconductor or to interlevel vias, as long as there is good adhesion, a stress gradient will form as mass is transported. This stress gradient opposes the electromigration driving force, slowing the mass transport. It will increase until one of two things occurs. Either the steady state will be achieved, where the stress gradient produces a driving force equal and opposite to electromigration and mass flow stops, or the peak stress will reach the critical level. In the former case, the conductor becomes "immortal' and will never fail. In the latter case a void or an extrusion will be generated. Which occurs is a function of the length of the conductor, the boundary conditions and the initial stress state.

For any current density there will be a length of conductor below which failure cannot occur, called the "Blech Length". The product of this length and the current density is a constant (called the "Blech Product") which is a function of the conductor material. Given an initial stress free state (which never happens), it is on the order of a few thousand in units of A/cm for Al alloys. Thus at a typical use current density of a few hundred thousand amps/cm^2, any conductor less than about 100 μm long will never fail.

Unfortunately, thin films conductors are never initially stress free, but, due to the differences in the coefficients of thermal expansion between metal semiconductors, they are under a tensile stress. When confined by interlevel dielectric, the stresses are hydrostatic and VERY large, many times the normal engineering yield stress. Therefore, the critical failure stress may be nearly achieved by the thermal contraction before the current is turned on and it would take very little additional electromigration induced stress for damage to form. This shortens the time required to reach the critical stress as compared to a stress free material and also shortens the Blech Length. In fact the Blech Length can go to zero, a condition known as stress voiding.

The boundary conditions are also important. We can have two realistic conditions in ICs. Either we have both ends of the conductor experiencing blocking (J=0) boundary conditions, such as a line connecting one contact to another, or we have one end at J=0 and the other stress free, such as at a bond pad. It can be shown that the "one-ended" BC (bond pad to contact) is the worst case. The maximum stress at steady state for this configuration is exactly twice that of the other.

A third condition, where we have stress free boundary conditions at each end (bond pad to bond pad) only occurs in standardized test structures and are essentially irrelevant to reliability. The steady state stress for this configuration contains stress dipoles at local flux divergences. In a bamboo structure they don't exist and in a near-bamboo structure the stress dipoles are limited by the size of the fine-grain clusters. Therefore test structures of this type last much longer than more realistic geometries containing vias or contacts. Design rules based solely on results from NIST type structures may be dangerously aggressive.

When a void forms in a completely enclosed conductor, the boundary conditions instantaneously and radically change. The surface of a void cannot sustain a normal force, so the hydrostatic stress vanishes. When it does, the maximum steady state stress immediately doubles. Prior to the void formation, a stress gradient was being established that inhibited electromigration induced mass flow (incidentally this is the reason behind the $1/j^2$ dependence on failure times). As soon as we have a void, the stress gradient temporarily reverses, enhancing mass flow until the stress gradient re-establishes itself. During this time we have a period of inflationary void growth resulting in a rapid increase in resistance.

If there were a pre-existing stress void, the resistance vs. time characteristics are somewhat different. Instead of being relatively constant and increasing rapidly, the explosive void growth stage is bypassed. The void will grow pretty much at a constant rate until a steady state stress profile is reached when the resistance value saturates. The eventual void size is a function of the amount of thermal stress, the current density and the length of the conductor line. The failure kinetics are also growth, rather than nucleation dominated resulting in a 1/j failure time dependence. This is usually not good.

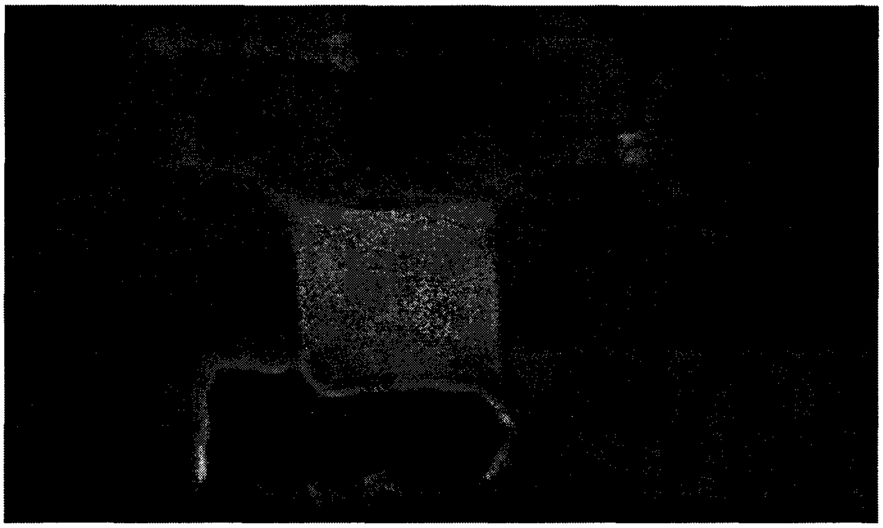

Fig.1 Typical electromigration induced void at a W via. The via provides the J=0 blocking boundary condition. The void volume is the sum of the thermal and the electromigration induced strain.

Effect of notches and poor step coverage

Edge defects (notches or mouse bites) and planar defects (step coverage) have been shown in the past to be significant reliability detractors. For submicron lines, however, the effects of such defects are much reduced. It should be pointed out that although the current density is raised at such defects, there is no associated flux divergence to first order. If we reduce the cross section by a factor of two we may be increasing the mobility accordingly, but the amount of material diffusing is correspondingly reduced so that the flux is unchanged. Only if there is a concomitant change in the diffusion pathway area will there be an issue.

For bamboo Al conductors a notch will not produce a flux divergence, but will raise the steady state stress value. The amount the stress will be raised is a function of the size of the defect, but the effect is generally quite small. Therefore narrow lines are relatively immune to the effects of notch type defects. For wider lines a notch may alter the grain boundary pathway network and produce a flux divergence.

The effect of poor step coverage is exactly the opposite. For wider lines, as long as poor step coverage doesn't produce Joule heating problems or alter the grain size, the effect is small. For narrow lines that are diffusing via interfacial diffusion, there may be an effect, depending on the primary interface. If the primary diffusion pathway is sidewall or lattice, there is no effect. If the primary diffusion pathway is the bottom or the top interface, thinning over steps can cause a flux divergence. The divergence will be relatively small, however, compared to, say, a contact, and the increase in steady state stress will also be small since the step coverage represents a very short length at high current density. Therefore, we come to the conclusion that poor step coverage is not much of an issue.

Bottom Line for Al Alloy Metallization

For contemporary submicron metallization the reliability is much better than expected from results with wider conductor lines. When the grain size is larger than the line width and bamboo structure conductors are achieved, Al based metallization is as much as an order of magnitude more reliable than wide lines at the same current density. Design rules should reflect this difference. Notch defects and poor step coverage are not major reliability concerns. Stress voiding can affect reliability and should be considered in reliability estimates and design rule generation.

Cu metallization

Until recently, copper metallization could be described as the material that "always was and always will be the wave of the future". This is in reference to its promise of low resistivity, better reliability yet difficult processing problems. Now it appears the processing challenges have been met, albeit with a complete change in the way we think about semiconductor manufacturing. The reliability issues, however, have not quite met the lofty expectations. (8,9)

Based on a rule of thumb that states that the activation energy for diffusion tracks with the melting temperature of a metal, one would expect Cu (T_m = 1063C) would experience much longer electromigration lifetimes than Al (T_m = 660C). What has been found, however, is that Cu metal does not have this anticipated advantage. Furthermore the increase in reliability with decreasing line width that was observed in Al/Cu metallization does not appear with Cu. As far as reliability is concerned, Cu has been something of a disappointment.

The reason for this is in the fundamental difference in the manner in which Al and Cu interact with their environment. Cu is one of the class of "Noble Metals" (Cu, Au and Ag) that are characterized by high conductivity, poor adhesion to most surfaces and resistance to oxidation. Al on the other hand is extremely reactive and adheres well to any oxidizing surface. As a result, any interface with Al is usually very "tight" and does not provide a pathway for rapid diffusion. In fact, interfacial diffusion in Al alloys is slower than in the grain boundary. For Cu, on the other hand, the interface is weak and diffusion on Cu interfaces is faster than in the grain boundaries.

As a consequence, the reliability of Cu is inversely proportional to the surface/interface to volume ratio of the conductor. The narrower the line, the worse the reliability. The microstructure also seems to have little or nothing to do with electromigration lifetime. In narrow lines, there is always more interface than grain boundary and since interfacial diffusion in Cu is faster than grain boundary diffusion, the grain structure is essentially irrelevant. Therefore, there is no increase in reliability as the line width becomes smaller than the grain size.

The activation energy for Cu interfacial diffusion is comparable to that for Al/Cu grain boundary diffusion, and less than Al/Cu interfacial diffusion. Therefore, Cu diffusion in narrow conductors is actually faster than in Al/Cu conductors despite the disparity in melting temperatures. In fact, it can be demonstrated that submicron Al alloy conductors are more reliable than comparable Cu conductors. (9)

The trick to making Cu reliable would then be to somehow tie up the interfaces so that mass transport would be forced to proceed via grain boundary or lattice diffusion. Experience has shown that this is a difficult, but not insurmountable, task. The literature is filled with highly variable experimental results showing that, if this is achievable, it is not very consistent. Like the limerick about the little girl with the curl in the middle of her forehead, when she (and Cu is a she, assigned by the ancients to the planet Venus) is good, she is very very good but when she is bad she is horrid. If the Cu surface and interfaces are tied up, Cu is much more reliable than Al alloys, but if not it is much worse.

Bottom Line for Cu conductors

Cu is not as good as one might think compared to Al due to the fundamentally different way it interacts with its environment. The reliability of Cu does not improve when the line width becomes less than the grain size as with Al, so for submicron applications Cu can be shown to be no more reliable than Al alloys, unless we can shut off the surface as a diffusion pathway. Unlike Al, where thermodynamics makes it easy to do this, Cu must be carefully handled. If the process is under control, Cu will behave very reliably, but, if not, Cu alloys may be less reliable than contemporary Al/Cu conductors. Therefore, Cu should be principally chosen for its low resistivity, not its resistance to electromigration.

The ancients ascribed supernatural qualities to the seven metals of antiquity (Cu, Ag, Au, Pb, Sn, Fe, Hg). Cu was assigned to the planet Venus, with feminine qualities. Therefore, it is not politically incorrect to refer to Cu as "she" and to recall a line of doggerel about the little girl with the curl in the middle of her forehead.

"When she was good, she was very very good, but when she was bad, she was horrid"

Low-k Dielectrics

Unfortunately the properties of low-k dielectrics that are of concern to reliability are diametrically opposed to its electrical properties. As the dielectric constant comes down, the diffusion coefficient for just about any metal goes up. This is also true for its permeability to water. Therefore, to achieve the low RC time constant we need for high performance circuits, we sacrifice its resistance to degradation from the operational environment. Hermetic packaging will be a must.

In addition, the thermal conductivity varies with k. The lower the k the less power we can dissipate in metal lines enclosed in the dielectric. This means less current can be carried without excessive Joule heating. Less current means a slower circuit. These considerations must be accounted for in the design rules and carefully checked in any qualification.

The problems are acute when using Cu. Even SiO_2, the traditional dielectric, is permeable to Cu. All one needs to do is glance at an Ellingham diagram to see the reason for the problems of Cu. (10) The Ellingham diagram displays the free energy of formation of a compound as a function of temperature. The free energy of oxide formation for Cu is relatively low, whereas for Al it is extremely high. Al is a rocket fuel. Therefore, if Al is in contact with just about any oxide it will reduce it and form Al_2O_3. Alumina is very tough, stable and refractory. It is therefore an excellent natural diffusion barrier and an adhesion promoter. Cu, on the other hand will not reduce any oxide of interest and in fact its own oxide will be reduced by any free metals that may exist in the dielectric. Therefore Cu will be free to diffuse atomically in virtually any material. Cu requires a perfect diffusion barrier to make it viable with any dielectric, and low-k dielectrics in particular.

Bottom line for low-k

Low-k and reliability do not go hand in hand. The properties of low-k dielectrics are diametrically opposed to reliability. Performance must be paid for in increased awareness to failure modes of corrosion, leakage and Joule heating. Cu is particularly susceptible to the problems of low-k dielectrics.

Summary

The reliability issues in both Cu and low-k dielectric technologies represent a fundamental shift from the traditional problems associated with IC manufacturing. The most important is that the fundamental chemical nature of Cu is very different from Al. Therefore, although significant improvements in IC design and performance can be realized with the use of Cu and low-k dielectrics, the manufacturing process will be much less forgiving than with older technologies and the reliability will have to be watched more closely.

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References

1) J.R. Lloyd, J. Phys. D. Appl. Phys. 32, R109 (1999) and references therein.
2) J.R. Lloyd, MRS Proc. Vol. 428, 3 (1996)
3) I. Ames, F.M. d'Heurle and R.E. Horstmann, IBM J. Res. And Dev. 14, 461 (1970)
4) M.J. Attardo and R. Rosenberg, J. Appl. Phys. 41, 2381 (1970)
5) S. Vaidya, T.T. Sheng and A.K. Sinha, Appl. Phys. Lett. 36, 464 (1980)
6) J. Cho and C.V. Thompson, Appl. Phys. Lett. 54, 2577 (1989)
7) J.R. Lloyd, Microelectronic Engineering 49, 51 (1999)
8) J.R. Lloyd and J.J. Clement, Thin Solid Films, 262 125 (1995)
9) H.J.T. Ellingham, Trans. Soc. Chem. Ind. 63, 125 (1944)
10) J.R. Lloyd, J. Clemens and R. Snede, Microelectron. Reliab., 39, 1595 (1999)