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Stress and dislocations in thin metal layers

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Stress and dislocations in thin metal layers

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Contents

Introduction

Since ancient times, metal has primarily served as a material for structural, load-bearing applications and for the fabrication of tools. Thus, the importance of the mechanical properties of metals has been recognized since many centuries. The strong interest in understanding the mechanical behavior of structural materials has led to much research and, to date, to an appreciably good knowledge of bulk metal behavior.

With the advent of the information revolution, metal has found a new field of applicability in the electronics industry. Integrated circuits and electronic devices make wide use of metal in the form of thin films and connecting wires. In such kind of applications, metal does not serve as structural material and seems to not have any load to bear. The same holds for all the other materials used in electronics. For this reason the mechanical properties of electronic components have been considered unimportant for quite a long time. Materials to be used, have always been selected on the basis of their electronic, magnetic or optical properties and not on the base of their mechanical reliability.

Quite unexpectedly, however, a significant number of electronic components turned out to fail mechanically, sometimes during operation and sometimes already during processing. Together with the overall tendency of making the devices smaller and smaller, the frequency of mechanical failure has increased. This observation has promoted extensive research on the mechanical behavior of small structures in the last few decades.

What has been found is that classical continuum plasticity is not applicable when at least one of the dimensions of the structure is in the micrometer range. When this happens, characteristic material length scales, such as the Burgers vector of the dislocation, dimensions related to dislocation patterning or to the microstructure, are not negligible anymore because they are comparable to the structure dimensions. These characteristic material lengths are related to strain and stress gradients which develop in the small structure when it is subjected to loading, in a way that is not well understood. Clearly, the dimensional constraint has an effect on plastic relaxation of small metal structures, like thin films. Several experiments have shown that thin metal films on a rigid substrate strengthen more than the corresponding bulk material. Moreover, with decreasing thickness the films show less and less plasticity. This phenomenon, frequently referred to as the thin film size effect, is still under investigation and this thesis is intended as a contribution to its understanding.

Thermal stress in thin films

Thermal stress is one of the main causes for the observed failure of electronic devices. In those structures, materials with very different elastic properties are packed closely together with deposition techniques that require high temperatures. During cooling to room temperature high thermal stresses develop because the various components have different thermal expansion coefficients. Plastic deformation in the metallic film can relax these stresses. Since plastic relaxation appears to be hindered in small metal structures, the residual stress present after manufacturing can be high enough to induce fracture or delamination of the thin metal films involved. Thermal stresses and relaxation also occur in service when devices are switched on or off.

When a thin metal film is thermally cycled on a rigid substrate, the imposed thermal strain is accommodated as elastic and plastic strain in the film, so that

$$\varepsilon_{\mathrm{thermal}} + \varepsilon_{\mathrm{elastic}} + \varepsilon_{\mathrm{plastic}} = 0, \tag{1}$$

where, for a change in temperature ΔT, the thermal strain can be written as

$$\varepsilon_{\mathrm{thermal}} = \Delta\alpha\Delta T. \tag{2}$$

Here $\Delta\alpha$ is the difference in the linear thermal expansion coefficients between the film and the substrate.

Let us assume that the film is elastic and isotropic. Since the film is thin, it can safely be assumed to be in a state of uniform plane stress, i.e.,

$$\sigma_{zz} = \sigma_{xz} = \sigma_{yz} = 0, \tag{3}$$

z being the direction normal to the film-substrate interface, while the in-plane principal stresses σ_x and σ_y are identical because of symmetry and $\sigma_{xy} = 0$. The elastic stress–strain relationship (Hooke's law) takes the simple form

$$\varepsilon_x = \varepsilon_y = \frac{1}{E}(\sigma_x - \nu\sigma_y), \tag{4}$$

with E being Young's modulus and ν Poisson's ratio. Since the thermal strain is also the same in x- and y-direction, the biaxial stress becomes

$$\sigma = \frac{E}{(1-\nu)} \Delta\alpha\Delta T. \tag{5}$$

Thus, in curves representing stress versus temperature the slope can never exceed the thermoelastic slope $[E/(1-\nu)]\Delta\alpha$. Deviation from the elastic slope gives a measure of plasticity in the film.

The stress in an elastic film is independent of film thickness. A dependence on thickness does also not appear by accounting for plasticity in the classical way. Yield functions do not depend on film thickness, neither do hardening laws. But, yield strength and hardening of real thin layers do, as we will see in the following section.

Experimental observation

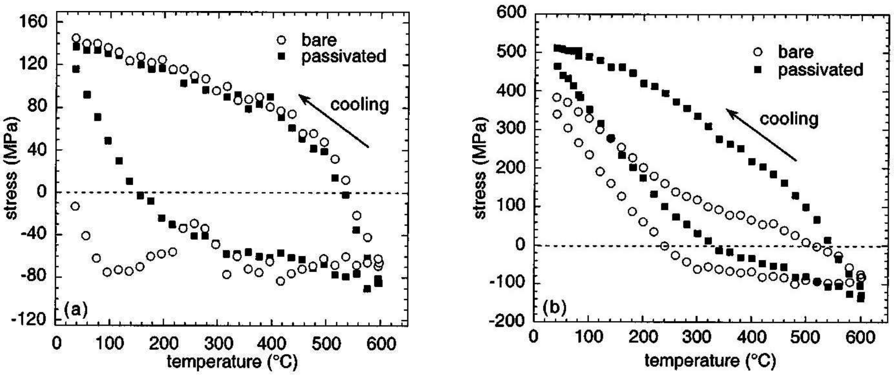
Figure 1 shows typical experimental stress–temperature curves for thin films under thermal cycling. Wafer curvature measurements have been performed on bare and passivated gold films on a silicon substrate. The figure shows that, after cooling by 600K, the biaxial stress in films of thickness $h = 0.75\mu$m (in Fig. 1a) is more relaxed than in films of thickness $h = 0.5\mu$m (in Fig. 1b). The presence of a passivation layer influences the behavior of the thinner film by increasing its hardness even further.

Experimental techniques

The traditional technique used to experimentally measure the stress in a thin film on a substrate is the wafer curvature technique. The method is based on the observation that the stress in the film exerts forces on the substrate that tend to bend the substrate elastically. By measuring the curvature of the substrate the biaxial stress in the film is calculated through Stoney's equation

$$\sigma = \frac{1}{6} \frac{E_s}{1-\nu_s} \frac{h_s}{h_f} \frac{h_s}{R}, \tag{6}$$

where h_s and h_f are the substrate and film thickness, R the substrate curvature. It should be noted that Stoney's equation does not contain the elastic constants of the



(a) (b)

Figure 1 Thermal cycling of gold films on silicon of thickness (a) $h = 0.75\mu$m and (b) $h = 0.5\mu$m (from [1]).

film, only those of the substrate (which are generally known). The influence of the film response is negligible as long as the thickness of the film is much smaller than the thickness of the substrate. Equation (6) is valid if the film deforms elastically and/or plastically, but obviously does not hold in case the substrate also becomes plastic.

Various techniques are available to measure the change in curvature; the most widely used ones are X-ray diffraction, optical interferometry and laser scanning. The wafer curvature technique is well-suited for in-situ stress measurements during heating and cooling of films and is commonly used to obtain stress–temperature curves. Since this is an indirect method, it only measures the average stress in the film, possible variations of the stress through the film thickness are not detected. In principle, X-ray diffraction would enable to see stress gradients across the film thickness by directly measuring the lattice strain in the film. Unfortunately the penetration depth of the beam cannot be tuned accurately and the presence of strain gradients across fractions of a micrometer are very difficult to detect. The most accurate technics in this respect are the glancing angle X-ray diffraction [2] and the energy-filtered electron diffraction techniques [3].

Freund-Nix model

Considering that stress relaxation in thin metal films occurs by dislocation glide, as shown experimentally for instance by Dehm et al. [4] (see Fig. 2), Freund [5] and Nix [6] proposed a model based on the motion of a single threading dislocation. Threading dislocations are dislocations that are present in the substrate before the film is deposited and grow naturally into the film during film growth by a glide and climb process, reaching the free surface. When stress develops in the film the part of threading dislocation in the film start to move, while the part in the substrate stays stationary. Thus, the dislocation bends over in the film as it moves and eventually leaves a misfit dislocation in the film. The minimum biaxial stress necessary to move a dislocation in the film, depositing dislocation length at the film–substrate interface, is given by

$$\sigma = \frac{\sin\phi}{\cos\phi\cos\lambda}\frac{b}{2\pi(1-\nu)h}\left[\frac{\mu_f\mu_s}{\mu_f+\mu_s}\ln\frac{\beta_s h}{b}\right], \tag{7}$$

where ϕ is the angle between the normal to the plane of the film and the normal to the glide plane, λ is the angle between the normal to the plane of the film and the Burgers vector b, and μ_f and μ_s are the elastic shear moduli of film and substrate. One of the key characteristics of the model is that it predicts that the stress is inversely proportional to the film thickness h.

The limitation of this model is that it only accounts for a single dislocation and its interaction with the interface. Since it neglects the effect of interaction among dislocations or between dislocations and other obstacles that might be present in the film, the model tends to underestimate the stress measured experimentally. For this reason, this thesis is concerned with the analysis of stress relaxation caused by the collective behavior of many dislocations. In addition to thin films, also interconnect lines are studied.

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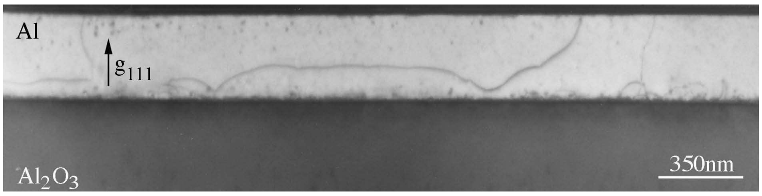

Figure 2 TEM image of a threading dislocation in a thin film (from [4]).

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