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Stress and dislocations in thin metal layers

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Document Version
Publisher's PDF, also known as Version of record

Publication date:
2004

Link to publication in University of Groningen/UMCG research database

Citation for published version (APA):
Nicola, L. (2004). *Stress and dislocations in thin metal layers*. [Thesis fully internal (DIV), Groningen]. s.n.

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Summary

According to experimental findings there are types of loading for which it is more difficult to plastically deform small metal structures than the corresponding massive metal. This occurs when at least one of the dimensions of the structure is at the micrometer scale or smaller. It is for instance the case of thin metal coatings: the thinner is the film, the more difficult it is to deform it plastically. This feature is in contrast with what expected on the basis of classical plasticity theories, which predict a size-*in*dependent mechanical response.

In this thesis the size effect in thin films is studied by means of two-dimensional discrete dislocation plasticity. Plasticity is treated as the collective motion of edge dislocations on prescribed slip systems. The framework contains an intrinsic length scale –the dislocation Burgers vector– which is a necessary condition to capture a size effect.

After a brief introduction of the method in the first chapter, attention is focused on the mechanical behavior of single crystal thin films on a large substrate (chapters 2 and 3). The practically relevant loading studied is that the film-substrate system is being subjected to a change in temperature. Tensile stress develops in the film during cooling, due to the difference in the coefficients of thermal expansion of film and substrate. Stress relaxation by plastic deformation in films that are between 0.25 and 1μm thick (chapter 2) is found to be dependent on this film thickness. The thickness dependence of the resulting film stress is in good qualitative agreement with the experimental findings. The origin of this size effect is the formation of a hard boundary layer comprising dislocation pile-ups at the film–substrate interface, which is modelled as impenetrable for the dislocations. Since the layer does not scale with film thickness, its contribution to the overall response increases with decreasing film thickness, hence giving rise to the size effect. Nevertheless, as shown in chapter 3, the boundary layer is not the only cause for the size effect in thin film: films thinner than a material-dependent threshold-thickness harden mainly because of insufficient nucleation activity.

Chapter 4 is devoted to the analysis of stress relaxation in single crystal metallic interconnects for integrated circuits. A cross–sectional analysis of the line is

carried out, with plane strain condition imposed in the direction along the line. The dependence of stress development and relaxation on line size and aspect ratio is explored. Stress relaxation by dislocation glide is not effective in lines with hight-to-width aspect ratio close to unity, for which the stress is almost hydrostatic. In lines with a smaller aspect ratio relaxation is quite effective in the center of the line, with dislocations forming boundary layers at the top and bottom of the interconnect. The presence of this boundary layers is responsible for a size effect in lines with a small cross-section.

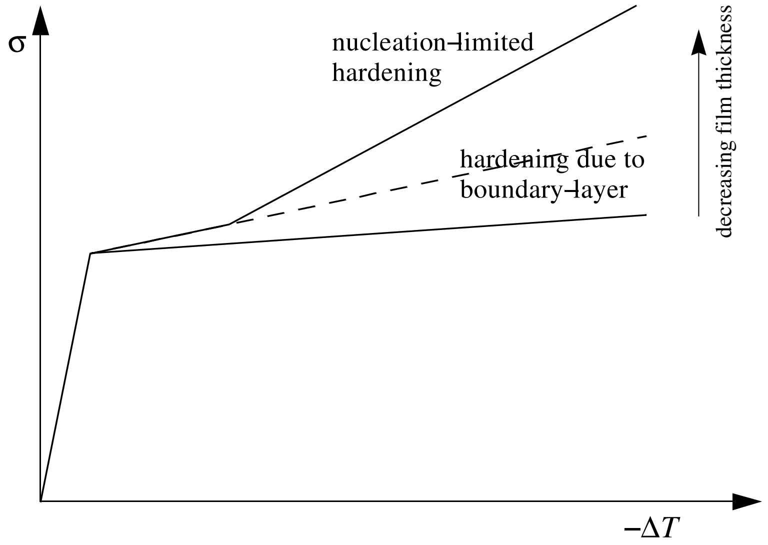

Figure 1 Schematic summary of the two hardening mechanisms found in crystalline thin films on a hard substrate. Average film stress is σ, temperature rise is ΔT.

In chapter 5 the thin film problem analyzed in chapters 2 and 3 is extended to polycrystalline films. The columnar grains, of which deposited films are generally made of, are modelled as rectangular single crystals of constant width. In this way a new length scale is introduced, i.e. the grain size, which gives an additional microstructural constraint to stress relaxation. The model permits to independently vary film thickness and grain size. The simulations show both film-thickness and grain-size dependent hardening. The latter is known in bulk as the Hall-Petch effect, but its scaling relation does not seem to apply to thin films.

An alternative to discrete dislocation plasticity is to develop a nonlocal version of standard continuum plasticity theory so as to introduce a material length scale. The form of such a theory is not known however, and several formulations can be found in the literature. In chapter 6 the strain gradient plasticity theory proposed by Gurtin [1] for single crystals is discussed. This theory attributes the nonlocal or gradient effect to the net Burgers vector of dislocations; this makes it well suitable for a comparison with discrete dislocation simulations. Different forms for the defect energy in the strain gradient theory are proposed and then used to solve the thin film problem of chapter 2. By comparing the solutions with the results of the simulations, it is possible to fit the length scales appearing in Gurtin's theory. The best fit is found for a defect energy that is proportional to the energy in dislocation pile-ups.

While all previous chapters dealt with films on a strong substrate, the last chapter supplements this with a study of free-standing thin films. Discrete dislocation simulations of such films under tension are confronted against experimental results in which grain size and film thickness are varied independently. The experimental work is carried out by Xiang and Vlassak [2] on a bulge testing machine, where the specimens are kept under plane strain conditions, which should support the assumption of a two-dimensional problem. Stress-strain curves show a size effect for passivated films of thickness ranging between 1 and 4.2 μm. Moreover, hardening is found to depend on the presence of passivation layers. The simulations are performed in order to reproduce the experimental curves by fitting two unknown parameters, namely the dislocation source density and strength.

References

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[2] Y. Xiang, J.J. Vlassak, M.T. Perez-Prado, Mat. Res. Soc. Symp. Proc., **795** (2003) paper U11.37.