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Stress and dislocations in thin metal layers

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Chapter 8

Discussion and outlook

The simple model presented in this thesis has proved to be capable of capturing thickness dependent hardening in thin metal films under tensile loading. What causes a size effect in these simulations is the formation of dislocation pile-ups at the interface between film and substrate (see chapters 2, 3 and 4) or film and coating (chapters 4 and 7). The back stress associated to these pile-ups has proved to be the major cause for thickness-dependent hardening (chapter 3).

The formation of a boundary layer has been shown to occur in films with a perfectly impenetrable interface with the substrate (or coating) while it does not occur if the interface is perfectly absorbing (see chapter 3). A more realistic view of the formation of a boundary layer could be obtained by modelling the interface as being partially capable to absorb dislocations, as in the case of an interphase. The numerical difficulty that arises when dislocations penetrate the substrate is the proper treatment of the displacement step that each dislocation would leave.

A similar remark can be made about grain boundaries in polycrystalline films: modeling them as impenetrable, flat and unidimensional (in two dimensions) is restrictive. In case the boundary were partially penetrable, the grain–size dependent hardening found in chapter 5 would probably be less pronounced. The difficulty in modelling partially penetrable grain boundaries in this framework is in the fact that dislocations, by moving from one grain into another, must climb on a slip plane with different orientation.

A difference in the interface boundary layer as well as in the surface boundary layer found for polycrystalline films with small grains (see chapter 5) can be expected if nucleation from interface and free surface were accounted for. By modelling generation of a new dislocation loop as a dislocation pair at the nucleation distance L_{nuc} (see chapter 1), the sources need to be placed at a distance $\frac{1}{2}L_{\mathrm{nuc}}\sin\phi$ from interface or surface in order for the freshly generated couple to be contained inside the film. Therefore, there is a thin layer close to interface, free surface and grain boundary where dislocation sources are absent. If sources were present also there, the boundary layer would be less uniform and the size effect less pronounced.

The effect of having nucleation partly occurring from the interface, the surface and grain boundaries would very likely only decrease hardening, so that the size effect would simply shift to smaller film thickness. Nevertheless, since experiments and molecular dynamics simulations suggest that nucleation in thin films occurs predominantly from grain boundaries and interfaces, it would be interesting to model sources accordingly, since this could affect the results of the simulations substantially.

What is certainly missing in this model are three-dimensional effects, such as line tension and dynamic formation of dislocation entanglements. In the present two-dimensional model dislocations form entanglements only if their edge parts meet in the plane of deformation. Interactions of dislocations on other planes are not accounted for. This is evident in the results of the simulation of the unpassivated freestanding thin film presented in chapter 7, for which hardening never occurs. Three-dimensional discrete dislocation plasticity models would be more appropriate to address this problem, or at least a two-dimensional model as the one proposed by Benzerga et al. [1], where three-dimensional effects are partly incorporated. With such a model, hardening of unpassivated films could be captured for a large enough strain, by increasing the density of forest dislocations during deformation.

Three-dimensional discrete dislocation plasticity simulations are at present computationally very expensive, due to the difficulty in treating the boundary conditions and the complicated line shapes and interactions [2]. In addition, the number of mechanisms included and numerical algorithms involved, makes the interpretation of the results quite difficult and may not add to a significant improvement of understanding.

References

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