

ATOMISTIC AND CONTINUUM STUDIES OF CRACK-LIKE DIFFUSION WEDGES AND DISLOCATIONS IN SUBMICRON THIN FILMS

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Recently developed theory of diffusional creep in thin metallic films constrained by substrates has identified a new class of defects called grain boundary diffusion wedges. These diffusion wedges are formed by stress driven mass transport between the free surface of the film and the grain boundary (GB) during the process of substrate-constrained grain boundary diffusion. An important implication of the theoretical analysis is that dislocations with Burgers vector parallel to the interface can be nucleated at the root of the GB. This is a new dislocation mechanism in thin films which contrasts to the well-known Mathews-Freund-Nix mechanism of threading dislocation propagation. Recent TEM experiments at the Max Planck Institute have shown that, while threading dislocations dominate in passivated metal films, parallel glide (PG) dislocations dominate in unpassivated copper films with thickness below 200 nm. Understanding the role of dislocations in submicron thin films from the atomistic viewpoint remains an open question. It is thought to be characterized by a complex interplay of diffusion, dislocation motion and resulting mechanical properties. Guided by the theory and the experimental results, we propose large-scale atomistic modeling of constrained diffusional creep to investigate this complex interplay from a fundamental perspective.

Our simulations suggest that nucleation of parallel glide dislocations competes with the “classical” threading dislocation mechanism and is coupled to diffusion activity. The atomistic modeling reveals that mass transport along the grain boundary leads to a stress relaxation in the film. The mass accumulation in the GB is interpreted as a pileup of climb dislocations, and leads to a crack-like stress concentration at the interface of film and substrate. This causes nucleation of dislocations with Burgers vector parallel to the interface, if the local dislocation density exceeds a threshold value. We present a detailed atomistic analysis of constrained diffusional creep and subsequent dislocation nucleation process. Atomistic simulations guide us to develop a criterion for a critical condition for initiation of diffusion. We compare nucleation of dislocations from a crack with nucleation from a diffusion wedge, and calculate a critical stress intensity factor (SIF) for dislocation nucleation from the atomistic data in both cases. In the spirit of the Rice-Thomson model, we develop a nucleation criterion for dislocation nucleation from a diffusion wedge. The theoretical prediction for critical SIF and the critical SIF from atomistic data show good agreement. Calculation of stresses in the film from atomistic data enables to investigate the film thickness dependence of characteristic time for stress decay. We find a scaling of characteristic time with film thickness to be $\eta \approx 2.65$, being close to the continuum theory prediction of $\eta^{CT} = 3$ (Coble creep). This study closes the theory-experiment-simulation linkage.

References

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