8.1 Modeling Concurrent Radiation Damage and Plastic Deformation[1] — T. Crosby, G. Po, N. Ghoniem (University of California, Los Angeles)

OBJECTIVE

This work has as an objective the modeling of concurrent radiation damage and plastic deformation in irradiated materials using a newly developed dislocation dynamics.

SUMMARY

We present here an application of a fundamentally new theoretical framework for description of the simultaneous evolution of radiation damage and plasticity that can describe both in-situ and ex-situ deformation of structural materials. The developed self-consistent framework allows for the determination of the simultaneous evolution of the dislocation microstructure, as well as the spatial distribution of vacancies, interstitials and the temperature diffusion fields. The developed theory is implemented in a new computational code that facilitates the simulation of irradiated and unirradiated materials alike in a consistent fashion. Computer simulations are presented for irradiated fcc metals that address dislocation channel formation in irradiated metals (ex-situ). The simulations, which focus on plastic flow localization in micro-pillars, show that the spatial heterogeneity in the distribution of Stacking Fault Tetrahedra (SFTs) leads to localize plastic deformation and incipient surface fracture of micropillars.

PROGRESS AND STATUS

Introduction

Irradiation of metals with high-energy particles, such as neutrons and ions, induces changes in the material microstructure and results in degradation of their mechanical properties. This has been well established and observed in experiments [1]. In low stacking-fault metals, such as Cu, the prevalent irradiation-induced defect is the vacancy-type stacking-fault tetrahedron (SFT) [2]. Depending on the fluence and energy of irradiated particles, the typical density of SFTs in irradiated fcc metals ranges between 10^{21} – 10^{24} m^{-3} [3]. The change in mechanical properties is manifest as an increase in the yield strength and a decrease in ductility. These changes are due to the fact that SFTs act as obstacles to the free glide of dislocation segments, causing them to be pinned at SFT sites. An increase in the applied stress is required to either break the dislocation free from the trapped configuration at the SFT site, or cut through the SFT and partially destroy it. A consequence of the physics of dislocation-SFT interaction is the onset of mechanical instabilities, such as plastic flow localization by forming defect free channels. This is attributed to dislocations absorbing SFTs, clearing paths for subsequent dislocations to glide freely, eventually creating defect-free dislocation deformation channels. Several numerical simulations showing the effect of SFT on the yield point and the interaction between dislocation segments and SFT have been reported in the literature, including atomistic simulations, discrete dislocation dynamics, and continuum dislocation dynamics. However, in these studies did not account for the effects of external surfaces on the onset of flow localization, nor did they consider the phenomenon in small-scale specimens, such as what is now commonly tested as micropillars.

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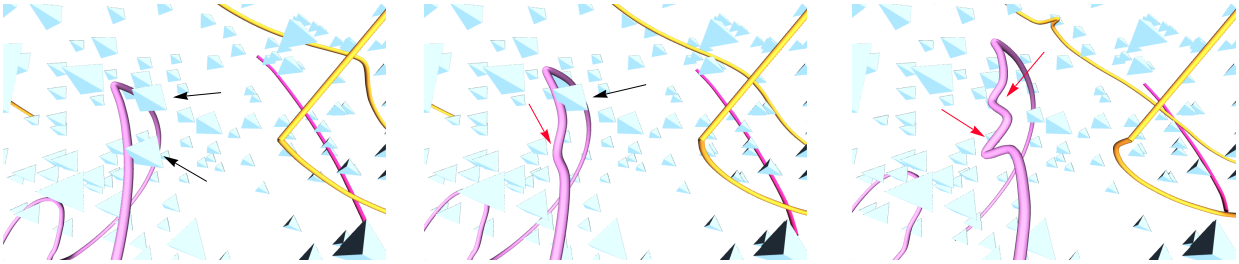
[1] A manuscript with the same title has been submitted to Journal of Nuclear Materials in October 2013.

RESULTS

Here, we model a Cu single crystal prismatic micropillar with a base of 250x250 nm and aspect ratio of 4:1. The pillar's bottom is fixed while its top surface is displaced with a fixed strain rate of 50 [1/s]. The lateral surfaces are free. The microstructure inside the pillar consists of dislocation segments and SFTs. The initial distribution of dislocations is generated randomly on all the 12 possible systems for fcc materials. The SFTs are randomly seeded inside the pillar following a uniform distribution. Image forces on the boundaries of the pillar are accounted for by coupling the DD method with elastic "correction" boundary value problem (bvp) and solved simultaneously. Due to the external and mutual stress, dislocations start to expand to form networks and interact forming junctions. During their motion, dislocation segments are randomly pinned at SFTs (Figure1a). When enough local stress is accumulated, a dislocation can overcome the SFT obstacle. In the process, SFTs may be destroyed according to a cumulative probability (Figure1c). Eventually a channel free of defects is formed (Figure 2). As a result, the glide of subsequent dislocations requires a lower applied stress.



(a) (b) (c)

Fig. 1. Interaction between a dislocation segment and two SFTs. The dislocation segment is initially pinned at their location. Eventually, the two SFTs are destroyed, and the segment is freed.

The model showed the formation of localized channels with low SFT defect density, high dislocation flux, and localized plastic distortion. As expected, the boundary plays an important role in breaking the symmetry of channel formation due to the mutual interaction between dislocation segments and the confined domain. This study can be furthered in the future by extending this framework to model polycrystalline materials with focus on crack initiation due to flow localization at grain boundaries. The study is also predictive, and awaits experimental validation, where neutron or ion irradiated copper micro-pillars can be fabricated and mechanically tested ex-situ.

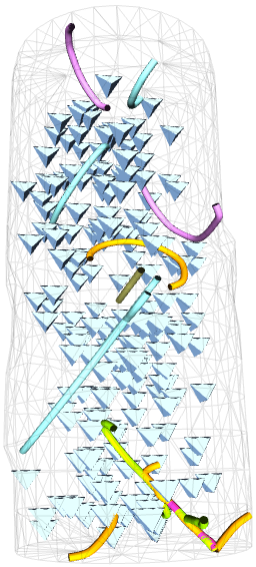


Fig. 2. Microstructure and channel formation.

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