3-D DISLOCATION DYNAMICS STUDY OF PLASTIC INSTABILITY IN IRRADIATED COPPER – L. Sun, N.M. Ghoniem, and B.N. Singh (University of California at Los Angeles)

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Extended Abstract

Experimental results consistently show that neutron irradiation of metals and alloys at temperatures below recovery stage V causes substantial increase in the upper yield stress and induces yield drop and plastic instability. Commonly, irradiated metals exhibit yield drop (following the upper yield point), do not show any work hardening and in many cases even show work softening. This specific type of plastic flow localization is considered to be one of many possibilities of plastic instabilities treated in the literature. At the upper yield point, plastic deformation is likely to be initiated in a localized fashion at sites acting as dislocation sources in the form of slip bands. These sites could be the locked dislocations themselves, or where the applied stress is intensified (e.g. grain boundaries, inclusions, triple points, etc.). It is important to recognize that when dislocation sources become operative initiating plastic deformation in a localized fashion, the whole specimen is strained at a very high level of applied stress. High velocity dislocations thus generated at sources may cut through soft and incoherent precipitates, or destroy previously built-up dislocation structures, causing softening in the active slip plane. Following neutron irradiation, the yield drop is observed to occur in pure FCC, BCC and HCP metals and alloys, provided that they are irradiated and tested at temperatures below recovery stage V. Recently, it has been proposed that the phenomenon of yield drop is caused by decoration of grown-in dislocations by small clusters or loops of Self-Interstitial Atoms (SIAs) produced in displacement cascades. Consequently, dislocations are immobilized, in a manner similar to that in the case of dislocations with an "atmosphere" of impurities or solute atoms in un-irradiated iron or Cu-30% Zn alloy. It has been shown that the decoration of dislocations by small SIA clusters is likely to occur, but only under cascade damage conditions where small glissile clusters are produced in displacement cascades. Investigations of post-deformation microstructure of irradiated metals and alloys have provided evidence for the formation of "cleared" channels. Virtually, all plastic deformation seems to occur in these channels representing only a small fraction of the specimens' volume. In the volume between these channels no dislocations are created during deformation. Once fresh dislocations are generated, they move very fast on their glide planes and cut, absorb or sweep irradiation-induced defect clusters and loops present on the glide plane. Consequently, cleared channels become almost defect free and thereby soft material for dislocation transport. This reinforces plastic strain localization and induces instability in plastic flow.

The onset of plastic instability in neutron-irradiated copper is investigated. Small prismatic defect clusters produced directly from collision cascades are trapped in the stress field of slip dislocations. Mobile prismatic clusters are absorbed in the dislocation core, when they approach within *~6 nm* as a result of torque-induced changes in their Burgers vector. Sessile vacancy clusters are also absorbed within this *"stand-off"* distance because of an induced surface tension on their stacking fault. The interaction between non-coplanar prismatic defect clusters and slip dislocations is shown to provide significant resistance to plastic deformation in irradiated copper. Coplanar sessile stacking fault tetrahedra and/or interstitial loops can additionally resist dislocation motion by localized forces on the glide plane before they are absorbed by activated dislocation sources. The comparison of the present results with experimentally measured yield stress of neutron-irradiated copper suggests that the plastic instability is most likely to be initiated at sites of stress concentrations.

Under irradiation, dislocation loops in copper are shown to attract small defect clusters. The size of the elastic capture zone is primarily determined by the interaction between the edge components of slip loops. At room temperature, calculated trapping zone sizes are on the order of 18 *nm*. Clusters which are produced closer than a "stand-off" distance of ~ 6 *nm* from the dislocation core are absorbed, either due to a high torque on their habit plane or due to unfaulting of small Frank loops. Recent MD calculations confirm that isotropic elasticity estimates for interaction energies are valid to within a few *nm* from the dislocation core. The flow shear stress required to unlock and push decorated dislocations on the glide plane is estimated to be above ~200-250 MPa for the passage of the first dislocation loop at the saturation level of hardening (i.e. dose > 10^{-3} *dpa*). This value is determined from elastic calculations for the interaction forces between the dislocation and defect clusters, and is somewhat lower than the estimates given in. The basic difference is in using somewhat lower values for average inter-cluster spacing and the standoff distance in. Most of the contributions to the resistive motion of slip dislocations are produced from nearby clusters close to the "stand-off" distance from the dislocation core. Once the dislocation is unlocked from its immediate surrounding clusters, it propagates on the slip plane by interaction and absorption of prismatic loops and SFT's. Beyond the upper yield point, the required shear stress is smaller, on the order of ~185 MPa. Since the experimentally measured tensile hardening value is about 250 MPa (with a maximum CRSS value of 125 MPa), we conclude that the initiation of flow instability is triggered by a stress concentration within the crystal. Even if a particular slip orientation with a Schmidt factor near 0.5 were selected within the crystal, the operating shear stress would still exceed the applied shear stress component by almost a factor of ~2. The current results predict that the orientations of flow localization are determined by the maximum possible value of the Schmidt factor, and that flow localization is most likely to occur in a region of stress concentration, such as an internal interface, inhomogeniety or an external surface. These results clearly demonstrate that while calculating the resistance to dislocation motion, the influence of both coplanar and non-coplanar loops and SFTs must be considered. Consideration of only coplanar obstacles underestimates the magnitude of radiation hardening, and does not account for the occurrence of the plastic instability.

FUTURE DIRECTIONS

Future research efforts will be directed towards computer modeling of various physical mechanisms that control flow localization and plastic instabilities in irradiated materials. We also plan to pursue the development and application of a comprehensive microstructure evolution, rate theory model, which accounts for the effects of helium and alloying elements.