**INVESTIGATIONS OF RADIATION HARDENING AND PLASTIC INSTABILITY IN FCC METALS** – N.M. Ghoniem, L. Z. Sun, B.N. Singh, and S.- H. Tong (University of California at Los Angeles)

Journal: *Phil. Mag.*, submitted, (1999)

Extended Abstract

A sudden transition of state from homogeneous plasticity to a mode of localized deformation is observed in many irradiated and unirradiated materials. This transition is considered to be a consequence of dislocation pinning with nano-scale barriers, such as solute atom atmospheres in unirradiated materials, or defect clusters in irradiated materials. The mechanism of flow localization and post-yield softening is investigated using a computational model of Dislocation Dynamics (DD). Radiation hardening and the onset of plastic instability in FCC metals, irradiated at temperatures below the recovery stage V, are analyzed in terms of three sequential pre-requisites:

trapping of mobile defect clusters during irradiation, leading to dislocation decoration and pinning;
post-irradiation activation of dislocation sources at regions of high stress concentration, such as grain boundaries, surface irregularities or inclusion interfaces;
penetration of activated dislocations through a system of defect barriers, destroying their resistance to subsequent dislocation glide.

A necessary condition for flow localization is a sudden release of large numbers of dislocations, which leads to a *negative* work hardening rate associated with defect cluster destruction. It is shown that irradiation-induced defect clusters in Cu are highly resistive to dislocation motion. At room temperature, stress concentration appears to be required for initiating plastic instability in copper at neutron fluence $10^{-3}$ dpa. It is also shown that the most likely orientations for dislocation channels are along slip directions of maximum Schmidt factors.

Most experiments on radiation hardening have been fitted to this simple form, showing that the increase in the yield strength scales as $\sqrt{\phi t}$ where $\phi t$ is the fast neutron fluence. In this scaling, the obstacles are all produced from collision cascades, and are approximately of the same size. Fitting to experimental data on irradiated metals has been used to determine the parameter $\alpha$ as an indication of the interaction mechanism (i.e. obstacle strength). It is found that $\alpha$~0.1 for irradiated Pd, and for irradiated Cu. Unfortunately, there appears to be a *fluence* dependence of $\alpha$ in the case of Cu, irradiated by 14 MeV neutrons, starting from a very low value of $\alpha$~0.04 at $\varphi t = 10^{20}$ n/m$^2$ to a higher value of $\alpha$~0.2 at $\varphi t > 2 \times 10^{21}$ n/m$^2$. An apparent abrupt change in the value of $\alpha$ occurs around a fluence of $\varphi t \sim 6\text{-}8 \times 10^{20}$ n/m$^2$. Furthermore, a different hardening rate was observed when Cu single crystal measurements were compared with polycrystalline results. Kojima, Zinkle and Heinisch (1991) observed that the low fluence dependence does not scale with $\sqrt{\phi t}$, and that there appears to be a mechanistic difference between low and high fluence results. Because of the difficulties in ascribing a single hardening mechanism, the experimental data of Mitchell (1978) were re-interpreted by Kojima, Zinkle and Heinisch (1991). The yield stress was linearly fitted with $\sqrt{\phi t}$, and shown to have a negative intercept of ~ (-22 MPa) at the origin. This was attributed to the Hall-Petch effect of grain boundaries in polycrytalline Cu, which is absent in single crystals. The obstacle strength parameter $\alpha$ obtained this way is ~ 0.23, which was concluded to be much smaller than the value proposed by Makin

(1968). If the Pd data of Baluc, Dai and Victoria are fitted in the same manner, without being forced to go through the origin, a positive intercept at the origin of ~ (+20 MPa) is obtained, in contrast with the analysis of Kojima, Zinkle and Heinisch (1991).

The objective of the present study is to assess the mechanisms responsible for the occurrence of plastic instability in irradiated FCC metals. In particular, we apply a new model of 3-D dislocation dynamics to analyze the interaction of slip dislocation loops with {\it both} coplanar and non-coplanar defect clusters in irradiated Cu. The investigation is aimed at explaining the specific mechanisms responsible for hardening in FCC metals and the origin of subsequent softening beyond the upper yield point. The present model extends the concept of CISH by providing detailed and quantitative determination of the increase in the yield stress of Cu under irradiation. We also introduce a new mechanism of post-yield softening, which was not considered in the original CISH model. The results of the present calculations are compared with the experimental data of irradiated copper (Singh, Edwards & Toft 1996), to show that the post-irradiation deformation behavior is controlled by the operation of a small number of dislocation sources that are highly stressed. This view is different from conventional hardening models which assume that {\it all dislocation sources} will operate at the yield point. The physical basis for the onset of plastic instability is discussed next, while we briefly outline our computational method for the simulation of mesoscopic plastic deformation of materials. Since dislocation generation and interaction with other defects dictate the initiation of plastic instability in irradiated materials, we give results of calculations for interaction energetics. Computer simulations for unlocking of slip dislocation loops, opposed by the long-range elastic field of random defect clusters are provided. Slip dislocations also interact with SFT's and sessile dislocation loops on their glide plane.

Under irradiation, dislocation loops in copper attract and trap nano-size glissile interstitial clusters. The size of the elastic capture zone is primarily determined by the interaction between the edge components of slip loops. Calculated trapping zone sizes at room temperature are 18 nm. Clusters which are produced closer than a distance of ~ 3-9 nm from the dislocation core are absorbed, either because of a high torque on their habit plane or by unfaulting of small Frank loops. It is shown that dislocations will be decorated with small defect clusters, which are trapped in their stress field, and are situated at a minimum stand-off distance. Thus, a natural length scale is realized before samples are subjected to a stress state during subsequent post-irradiation mechanical testing. The density of clusters in the immediate vicinity of locked dislocations is thus well above the background random density in the matrix. Our analysis of the required CRSS to unlock dislocations from an atmosphere of cluster density $10^{24}$ $m^{-3}$ shows that it is on the order of 200 MPa in Cu at RT. This is similar to the value calculated analytically by Singh et al. (1997) and Trinkaus et al. (1997b). It is concluded, therefore, that a higher CRSS is required to unlock dislocations from their cluster atmospheres. Since the measured value of the tensile stress increase because of neutron radiation is 250$ MPa at RT, it is concluded that the initiation of plastic flow within dislocation channels will most likely occur near regions of stress concentrations. 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 value. It is also possible that dislocations, which are not heavily decorated, will unlock from their defect atmosphere first without the necessity of a stress concentration. However, if a region in the crystal is near a stress raiser (e.g. precipitate, grain boundary, triple point junction, or surface irregularity), it is most likely that this site will yield first, and will result in flow localization. The directions of slip in localized flow regions are selected along the maximum possible values of the local Schmidt factor. Beyond the upper yield point, dislocation sources will operate by developing segments on the glide plane, which negotiate their way through a field of co-planar obstacles. Nevertheless, it is shown that the required CRSS in this case is less than that for

unlocking the dislocation from its surrounding cluster atmosphere. Once the first loop destroys opposing co-planar obstacles on the glide plane, emission of subsequent F-R loops becomes easy. The stress required for continuing the operation of the F-R source is determined by the normal forest hardening, and/or graining boundary pileup mechanisms, which generally require a smaller value of the CRSS.