DISLOCATION DECORATION WITH NANO-SCALE DEFECT CLUSTERS IN IRRADIATED METALS – N.M. Ghoniem, B. N. Singh, L. Z. Sun, and T. Diaz de la Rubia (University of California at Los Angeles)

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Extended Abstract

Accumulation of nano-size prismatic defect clusters near slip-dislocations results from their mutual elastic interaction. We present here 3-D isotropic elasticity calculations for the interaction energy between radiation-induced nano-size prismatic loops and grown-in dislocation loops. The current treatment extends the work of Trinkaus, Singh and Foreman in two respects. First, a computational method for a full 3-D analysis of interaction energies in BCC Fe and FCC Cu is developed. Second, the theoretical method of Kroupa is computationally implemented for rigorous calculations of force, torque and induced surface energy on defect clusters. It is shown that small clusters are trapped within a zone of ~10 *nm* in BCC Fe, and ~20 *nm* in FCC Cu at room temperature, in rough agreement with experimental observations. Clusters can be absorbed in the core of grown-in dislocations because of unbalanced moments, which provide sufficient energy for rotation of their Burgers vectors in a zone of 2~3 *nm* in Fe. Near the dislocation core (within a few nanometers), sessile defect clusters in Cu are shown to convert to a glissile configuration.

The present study reveals new features of defect cluster interaction with slip dislocations, and is thus complementary to the original work of Trinkaus, Singh and Foreman. The interaction between nano-size defect clusters and slip loops is shown to be highly orientation dependent, unlike the situation with point defects represented as centers of dilatation in calculations of dislocation bias factors. The size of the elastic capture zone is primarily determined by the interaction between the edge components of slip loops, and is not very sensitive to cluster-cluster interaction. Calculated trapping zone sizes are in reasonable agreement with experimental observations. In BCC crystals, unique interaction energy iso-surfaces for only four independent cluster orientations have been identified. These correspond to clusters with Burgers vectors of the type: $<111>$ $<\bar{1}11>$ $<\bar{1}\bar{1}1>$, and $<\bar{1}1\bar{1}$. Since cluster mobility is constrained by their glide cylinders, the elastic field of slip dislocations can only trap them, if their glide cylinders intersect with energy iso-surfaces whose level is more attractive than cluster thermal energy. Because of this directed motion in BCC crystals, clusters will tend to accumulate just below and above the slip plane, depending on their Burgers vector orientation, and on the character of the adjacent dislocation segment. Maximum cluster trapping is shown to occur near the edge component of a slip loop, while the trapping zone size decreases to zero near purely screw components. It is therefore expected that upon mechanical loading, edge components will be held up by clusters, while screw components will be free to move on the slip plane by glide and out of the plane by cross-slip.

It is also shown that clusters, which are very near dislocation cores (within ~*3 nm*) can be absorbed into the core by rotation of their Burgers vector as a result of unbalanced torque exerted on them by slip dislocations. If such clusters change the direction of their Burgers vector, they will move toward the dislocation core, and thus will possibly get absorbed. The dynamics of this final step can be ascertained by Molecular Dynamics (MD) atomistic studies of cluster incorporation into the dislocation core. The distance over which this scenario of cluster incorporation is estimated by the present method to be on the order of ~ *3 nm* for Fe at room temperature. Estimates for the size of the trapping and absorption zones are uncertain, because of the limitations of the model. It is not clear if there are significant effects of elastic anisotropy,

and large deformation close to the dislocation core, on the present results, which are obtained by linear isotropic elasticity. More accurate atomistic simulations may shed light on the inherent limitations of our model. It appears that the initiation of a dislocation channel on the slip plane is associated with the stress required for the dislocation to overcome the collective elastic potential of trapped clusters. This possibility is rather high in BCC crystals, and is a consequence of the high mobility of irradiation defect clusters. It remains to be seen, however, whether the plastic instability is initiated by *"absorption"* of small defect clusters, once they rotate their Burgers vector toward the dislocation core, or is a result of the leading dislocation *"sweeping"* these small clusters. The answer to this question may require dedicated experiments, as well as dynamical computer simulations. Both Molecular Dynamics (e.g. Ref. 20), and Dislocation Dynamics may be required to resolve this question. In either scenario, the type of radiation hardening appears to be of a "Cottrell" nature, similar to hardening by impurity clouds in alloys. This in contrast to hardening by dislocations cutting through dispersed barriers on the glide plane in the normal Orowan mechanism. Several features of cluster-dislocation interactions in FCC crystals are differentiated from the conclusions on BCC crystals. Small prismatic defect clusters in FCC crystals are sessile, because of the low stacking fault energy. They immediately dissociate into Schockley partial dislocations, with out-of-plane Burgers vector, rendering them sessile. However, we have shown that an *"induced surface tension"* is provided if clusters are nucleated near dislocation cores, or even if moving dislocations interact with them, thus altering the energy balance for their dissociation into partials. In either one of these two possibilities, dissociated, sessile clusters in FCC crystals may be converted to a glissile configuration. If these conditions were satisfied, it would potentially lead to the initiation of a plastic instability and the formation of clear channels. These scenarios remain tentative at present and need further analysis.