DISLOCATION DENSITY-BASED CONSTITUTIVE MODEL FOR THE MECHANICAL BEHAVIOR OF IRRADIATED CU—A. Arsenlis (Lawrence Livermore National Laboratory), B. D. Wirth (Department of Nuclear Engineering, University of California Berkeley), and M. Rhee (Lawrence Livermore National Laboratory)

EXTENDED ABSTRACT

Performance degradation of structural steels in nuclear environments results from the formation of a high number density of nanometer scale defects. The defects observed in copper-based alloys are composed of vacancy clusters in the form of stacking fault tetrahedra and/or prismatic dislocation loops that impede the motion of dislocations. The mechanical behavior of irradiated copper alloys exhibits increased yield strength, decreased total strain to failure and decreased work hardening as compared to their unirradiated behavior. Above certain critical defect concentrations (neutron doses), the mechanical behavior exhibits distinct upper yield points. In this paper, we describe the formulation of an internal state variable model for the mechanical behavior of such materials subject to these environments. This model has been developed within a multiscale materials modeling framework, in which molecular dynamics simulations of dislocation – radiation defect interactions inform the final coarse-grained continuum model. The plasticity model includes mechanisms for dislocation density growth and multiplication and for irradiation defect density evolution with dislocation interaction.

The material parameters for the constitutive model were fit to the published stress-strain behavior of unirradiated Cu, with irradiation damage-dependent constants approximated from the initial yield strength of irradiated Cu. We then compared model predictions of the homogeneous constitutive behavior to observed tensile stress-strain behavior of irradiated Cu, for variations of irradiation induced defect density between 4×10^{20} and 4×10^{23} m^{-3}, with an initial SFT size of 2.5 nm. The general behavior of the homogeneous constitutive model shows that as the defect density increases, the initial yield point increases and the initial strain hardening decreases. Implementation of the final coarse-grained constitutive model into a finite element framework was used to simulate the behavior of tensile specimens. The simulation results compare favorably with the experimentally observed mechanical behavior of irradiated Cu, and reproduce the increased strength, the decreased nominal strain at the ultimate tensile strength, the formation of an initial yield point forms above a critical SFT density of about 2×10^{23} m^{-3}, and higher stresses after the ultimate tensile strength for a given strain, as compared to unirradiated behavior.

Future modeling efforts will focus on coupling the constitutive model to a microstructure evolution model to predict the mechanical property changes as a function of irradiation variables and on developing a model for irradiated bcc alloys, which will require a temperature dependent dislocation velocity law to account for the inherent lattice resistance and the material's response to strain localization and the formation of adiabatic shear bands.

Reference

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