8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

MULTISCALE MODELING OF DEFORMATION AND FRACTURE OF STRUCTURAL MATERIALS IN NUCLEAR ENVIRONMENTS[i]

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Key Words: *Multiscale, deformation, fracture, nuclear materials, modeling.*

ABSTRACT

During the past few years, tremendous progress has been made in modeling and simulation of structural materials in severe irradiation environments. The main objective of this approach is to enable the development of radiation-resistant materials on physical and not empirical basis. In this presentation, we first discuss dislocation motion in irradiated materials, emphasizing unique aspects pertaining to the simultaneous climb and glide motion, interaction with Self Interstitial Atom (SIA) clusters and the influence of these interactions on dislocation mobility. We also highlight the pinning-depinning characteristics of dislocation movement under irradiation, the build-up of decorations around dislocations, the formation of SIA cluster "clouds" or "atmospheres" near dislocations, and the competitive process of "raft" formation as observed experimentally.

The effects of such interactions on the development of the dislocation microstructure during irradiation as opposed to post-irradiation will be discussed. Then we discuss recent efforts in modeling low-temperature embrittlement and fracture of ferritic/ martensitic steels and the shift in the Ductile-to-Brittle-Transition-Temperature (DBTT) by neutron irradiation. Efforts on modeling the deformation and fracture of coupled macro-micro cracks in irradiated steels will be also discussed. At the component length scale, we outline progress on the development of microstructure-based constitutive equations, their incorporation into plasticity models of deformation, and emphasize the critical role that crystal plasticity plays in understanding inhomogeneous plastic deformation and plastic instabilities. A global-local approach for coupling large-scale global Finite Element Modeling (FEM) to crystal plasticity analysis of local deformation at critical regions of fusion structures will be shown. We will finally discuss modeling challenges and limitations that face material scientists in developing radiation-resistant and robust structural materials and components for nuclear energy applications.

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[i] This work is supported by the U.S. Department of Energy, Office of Fusion Energy Science, and by the UCLA NERI Grant DE-FC07-06ID14748