Recent Advances in Multiscale Modeling of Deformation and Fracture

N. Ghoniem\textsuperscript{a}, B. Wirth\textsuperscript{b}, G. Odette\textsuperscript{c}, R.J. Kurtz\textsuperscript{d}, R. Stoller\textsuperscript{e}, S. Zinkle\textsuperscript{f}, Y. Osetskiy\textsuperscript{f} and S. Sharafat\textsuperscript{a}

\textsuperscript{a}Mechanical and Aerospace Engineering Department, UCLA, Los Angeles, AK CA-90095-1597, United States of America
\textsuperscript{b}Nuclear Engineering Department, UC, University of California, Berkeley, California, AK CA 94720-1730, United States of America
\textsuperscript{c}Department of Mechanical Engineering UCSB, UCSB, Santa-Barbara, AK 93106-5080, United States of America
\textsuperscript{d}Pacific Northwest National Laboratory, P.O. Box 999, Richland WA, AK 99352, United States of America
\textsuperscript{e}Materials Science and Technology Division, ORNL - Oak Ridge National Laboratory, P.O. Box 2008, Bldg 4500S - MS 6151, Oak Ridge, AK TN 37831-6151, United States of America
\textsuperscript{f}Materials Science and Technology Division, Oak Ridge National Laboratory, 1 Bethel Valley Rd., P.O. Box 2008, Oak Ridge, AK TN 37831-6138, United States of America
nghoniem@gmail.com

During the past few years, we have witnessed significant progress in modeling and simulation of fusion structural materials. In particular, the systematic approach of multiscale modeling has transformed our outlook towards the development of radiation-resistant materials from one that relies on empiricism to a robust, science-based process. First, we 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 aspects 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 delineate recent efforts in modeling low-temperature embrittlement of ferritic/martensitic steels and the shift in the Ductile-to-Brittle-Transition-Temperature (DBTT) by neutron irradiation. Progress on the Master Curve (MC) approach will be discussed to show how the uniqueness of the MC shape can be utilized to extract information on the controlling mechanism of dislocation mobility by kink-pair nucleation. Efforts on modeling the deformation and fracture of coupled macro-micro cracks in irradiated steels will also be 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 fusion materials and components.

This work is supported by the U.S. Department of Energy, Office of Fusion Energy Science

Number of words in abstract: 318
Keywords:
Technical area: 11. Multiscale modeling for fusion materials and structure
Special session: Not specified
Presentation: No preference
Special equipment: No special equipment