MODELING AND SIMULATION TECHNIQUES FOR STRUCTURAL MATERIALS UNDER FUSION CONDITIONS

J. Marian[1]

[1]*University of California, Los Angeles, USA*

Understanding and predicting the behavior of structural materials under fusion conditions requires the integration of modeling, experimentation, and validation across multiple length and time scales. Irradiation produces a series of chemical and microstructural changes in the material that profoundly alter its physical and mechanical properties, such as radiation hardening, loss of ductility, loss of thermal conductivity, and chemical transmutation. The lack of suitable surrogate fusion neutron sources points to theory, modeling, and simulation as an important tool to bridge the experimental gap posed by 14-MeV fusion neutrons sources and available testing facilities based on heavy ion beams or fission neutrons. Moreover, irradiation damage is initiated by particle collisions at the subatomic scale, but its effects are felt at the engineering level, This necessitates multiscale simulations capable of linking many orders of magnitude in time and length scales while quantifying uncertainties and guiding materials design.

The last decades have experienced substantial progress in terms of the accuracy, scale, and relevance of materials modeling under fusion reactor operation. Increasingly more complex and realistic material microstructures can now be simulated under fusion-representative conditions, complementing experiments and solidifying our understanding of materials behavior under meaningful dose rates, temperatures, gas atom-to-dpa ratios, and spectral details. As well, while many challenges still remain, the experience acquired by modeling teams over the last few decades has now resulted in a set of ‘best-practices? supported by a relatively wide community consensus with applications in a wide range of different operational scenarios. Current models can effectively capture irradiation damage buildup coupled to microstructural evolution, dose-rate and temperature dependent regimes, nuclear transmutation and gas atom evolution, solute mobilization by radiation enhanced diffusion, as well as the change in derivative quantities such as hardening, swelling, or creep. While important gaps in our understanding remain, particularly in terms of high dose and high temperature materials behavior, synergistic He/H effects in ferritic materials, pulsed irradiation, or chemical effects, we believe that modeling is presently in a good position to issue qualified materials behavior predictions in the anticipated operational range gap between a pilot fusion facility and suitable neutron sources. In particular, we will discuss potential differences in He- and H-to-dpa ratios, irradiation flux and pulsed regimes, probe volumes, and irradiation temperatures, as well as the potential implications of modeling long term transmutation-induced chemical composition changes, swelling, and creep. Finally, we will discuss the potential of new and improved techniques, including data-driven approaches, aided by an increased availability of computational resources, to push the envelope of our current understanding limits and improve error and uncertainty estimation of model predictions.