Contribution ID: **9** Type: **invited**

Sensitivity analysis and optimization of multi-scale models for microstructural evolution in metal materials under neutron irradiation

Tuesday 27 May 2025 14:20 (30 minutes)

Developing materials resistant to neutron irradiation is one of the key challenges in fusion energy applications. Due to the lack of fusion neutron sources for irradiation experiments, computational simulations provide valuable information and references for addressing such challenges. Multiscale simulation methods through a hierarchical, information-passing paradigm are often employed to study microstructural evolution of irradiated materials. Large-scale methods usually take the computational results of small-scale methods (such as Molecular Dynamics, MD) as input parameters. The uncertainties in small-scale methods can then propagate in large-scale methods, leading to inevitable uncertainties in the model predictions. In order to improve the accuracy of model predictions, it is necessary to perform parameter sensitivity analysis for multi-scale simulation methods.

This study conducted a sensitivity analysis on the Object Kinetic Monte Carlo (OKMC) simulations of tungsten (W) microstructural evolution under neutron irradiation. Initially, a total of 14 input parameters including capture radius, defect migration energies and pre-exponential factors were selected for analysis. The Latin hypercube sampling was used to construct the input space. The average size and number density of defect clusters were taken as quantity of interest (QoI), and the Spearman correlation coefficient was used as the sensitivity index. The results show that single-vacancy migration energy, self-interstitial rotation energy and capture radius are the most sensitive. These sensitive parameters were then characterized in a more accurate way to reduce model uncertainty and improve the accuracy of model predictions. For example, we performed a more accurate calculation of the capture radius of defects through molecular dynamics simulations. We used the optimized capture radius as the input parameter for OKMC simulations and found that the resulting average sizes and number densities of the defect clusters were in better agreement with the experimental results, confirming that the optimization of sensitive input parameters can improve the accuracy of OKMC model.

Primary author: YANG, Zhangcan (Huazhong University of Science and Technology)

Co-authors: Prof. ZHOU, Hong-Bo (Beihang University); Mr WAN, Shaoting (Huazhong University of Science and Technology)

Presenter: YANG, Zhangcan (Huazhong University of Science and Technology)

Session Classification: invited