Accelerating multiscale simulations of irradiated material properties using machine learning

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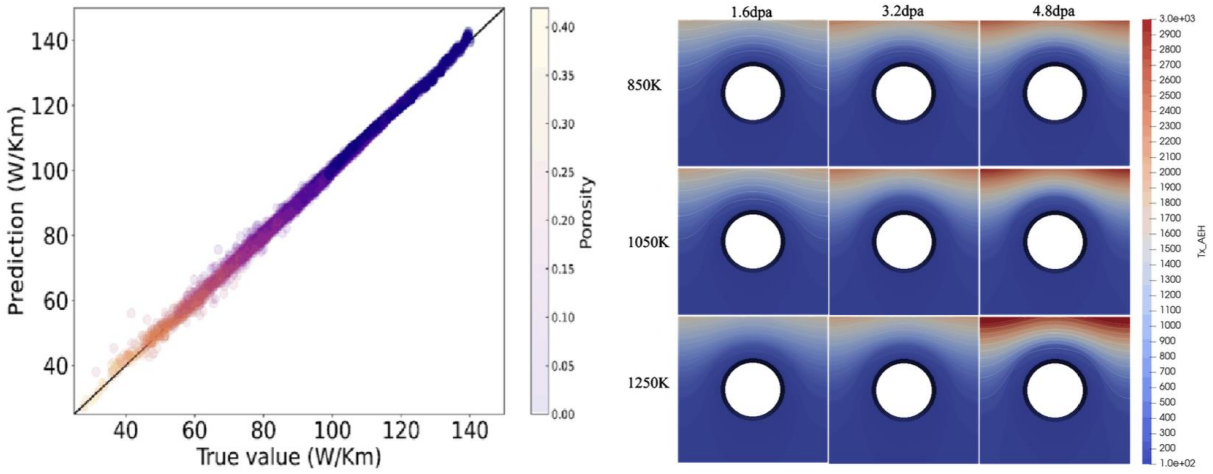
Abstract

Irradiation alerts materials across multiple scales, spanning from atomic processes and microstructural evolution to macroscopic property changes. Significant efforts have been made to develop multiscale simulations that establish the relationship between atomic structures and macroscopic properties. However, two key challenges hinder the effectiveness of such simulation. First, accurately and efficiently transferring information from low-scale to large-scale remains computationally demanding. Second, capturing the transient effects of irradiation environmental conditions on the evolution of defects at the low-scale simulation is complex and resource-intensive.

Recent advancements in machine learning techniques offer promising resolutions to mitigate these challenges. To this end, we propose a concurrent multiscale modelling framework that bridges atomic-scale and macroscopic scale simulation by utilizing machine-learning techniques to predict the thermal and mechanical properties of irradiated materials. We take the evolution of neutron irradiation in tungsten (W) as an example. The displacement cascades at a given energy are first simulated by the molecular dynamics (MD) method. These results are used to train the machine-learning model to predict the distribution of point defects within the PKA energy of 0-100 keV. Remarkably, it achieves a computational speedup of five orders of magnitude compared to MD simulations. The obtained defect structures are subsequently taken as input for the phase-field model to evolve at the diffusion time scale. By integrating a phase-field approach with the finite element method (FEM) to capture how microstructural changes affect macroscopic thermal and mechanical properties, i.e., effective thermal conductivity and

elastic modulus. To accelerate the phase-field simulations, we introduce a ResNet18-Long Short-Term Memory (LSTM) machine learning framework, incorporating phase-field microstructural information, significantly enhancing both computational speed and accuracy. the machine learning predicted effective thermal conductivities as input parameters are fed into macroscale FEM simulations, enabling an assessment of the temperature and stress distributions, and effective thermal conductivity and elastic modulus for macroscale W monoblocks. The machine learning aid multiscale simulation model provides an efficient and effective multi-scale simulation approach for understanding and predicting the evolutions of irradiation-induced defects to macroscopic properties in irradiated materials.

Keywords: multi-scale, machine learning, irradiation, defect evolutions, tungsten



(a) (b)

Fig. 1 (a) Comparison between phase-field calculated and machine-learning predicted values of effective thermal conductivities, where the horizontal axis represents phase-field calculated values and the vertical axis represents machine-learning predicted values. (b) Temperature distribution in a W monoblock under various thermal and dpa conditions. As heat flux increases, the overall temperature within the monoblock increases accordingly. With increasing dpa, a significant reduction in thermal conductivity is observed due to the accumulation of radiation-induced defects. This decrease in thermal conductivity limits the heat dissipation efficiency, resulting in localized heat buildup within the monoblock. Consequently, regions surrounding the central void exhibit elevated temperatures with increasing dpa, indicating that irradiation damage intensifies thermal stress in these areas.