Modeling Tutorial

From Ab Initio Models to a Virtual Tokamak Reactor: Fundamentals and Applications of Advanced Materials Modelling

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Under the operating conditions expected in demonstration magnetic fusion reactors beyond ITER, structural and plasma-facing materials will be exposed to unprecedented conditions of irradiation, heat flux, and stresses. While many of such extreme environments remain inaccessible to direct experiments, computational modeling and simulation can provide qualitative and quantitative insights into materials response, and complement the available experimental measurements with carefully validated predictions. The highly multiscale and multidisciplinary nature of materials evolution under fusion conditions calls for a wide-ranging treatment of physical processes from the subatomic scale to the component engineering length scale. These processes occur over timescales ranging from the very short timescales of 10^{-13} s characterizing atomic vibrations, to months and years. This extraordinary challenge has recently spurred tremendous advances in theory, modeling, and simulation, involving hundreds of researchers in institutions all over the world. In this tutorial, leading experts in the field will comprehensively cover the most important modeling techniques contributing to the multiscale paradigm, with special emphasis in how to inform engineering level models with fundamental physical information. The tutorial will provide the underlying mathematical background, show the fundamental connections linking the spatial and time scales, and give examples of experiments performed to validate the models.

The first lecture of the tutorial (Dudarev) will cover modern electronic structure methods with emphasis on simulations of defects and dislocations, atomistic simulations and their application to transport properties and dynamic displacement cascade simulations, and provide the elements of statistical mechanics and mathematical framework needed for connecting the microscopic models with microstructural evolution and macroscopic component level design. The second lecture (Marian) will focus on the evolution of the material microstructure under irradiation, both low-energy gas atom deposition and bulk fusion neutron exposure. Kinetic models such as mean-field rate theory, kinetic Monte Carlo, and accelerated molecular dynamics will be discussed in the context of irradiation damage accumulation to high doses and its effect on important properties such as dimensional stability, hardening, and embrittlement. The tutorial will conclude with a lecture (Po) on how to use microstructural information to evaluate mechanical properties using techniques such as dislocation dynamics, crystal plasticity, and thermodynamic modeling, and how to connect the above modelling approaches with finite element models for boundary value problems.

The tutorial will cover a broad range of materials, including W, as a material for plasma facing components Fe, Fe/Cr alloys, as important constituent elements of structural fusion steels. Also lectures will cover defect physics, microstructural evolution, and mechanical/dimensional property changes of materials exposed to fluxes of He/H isotopes as well as bulk materials subjected to fast neutron irradiation.

This tutorial will be open to registered ICFRM attendees free of charge. Lecture slides and tutorial materials will be provided to attendees.