DE LA RECHERCHE À L'INDUSTRIE

Séminaire

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Salle de réunion du SRMP – Bâtiment 520 - Pièce 109

Multi-Scale Modeling of Tungsten under Helium Irradiation

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In fusion reactors, plasma facing components (PFC), and in particular, the divertor will be irradiated with high fluxes (up to 10^{23} $m^{-2}s^{-1}$) of low energy (~ 100 eV) helium and hydrogen ions. Tungsten is one of the leading candidate materials for the divertor. However, the behaviour of Tungsten under high doses of helium exposure remains to be fully determined. Computational materials modeling has been used to investigate the mechanisms controlling microstructural evolution in Tungsten following high dose, high temperature helium exposure.

The aim of this talk is to present a framework to understand and predict defect production and diffusion, clustering and interaction close to the inner surface of the divertor due to high flux, low energy helium irradiation. The framework presented is based on a multi-scale approach: we present a spatially-dependent Cluster Dynamics (CD) model based on reaction-diffusion rate theory to describe the evolution in space and time of helium and its complexes. The processes modeled originate from both Molecular Dynamics (MD) observations at the atomistic scale and experimental results.

The use of cluster dynamics modeling suffers from physical as well as computational challenges: physical challenges due to the large number of physical quantities (diffusion coefficients and binding energies) to determine for each chemical species, and the applied mathematics and computational challenges due to the large number of species that are modeled. The CD model is parameterized using MD simulation results, and a solver was developed to efficiently deal with the large system of non-linear partial differential equations describing the microstructure evolution. The solver uses an algorithm designed to exploit the local structure of the chemical reactions and makes use of parallel computing to both speed-up computations and reduce the memory requirements per processor.

We compare the model with results from molecular dynamics simulations of helium cluster formation and evolution below the surface, results from experiments performed using thermal desorption spectroscopy, and results from experiments under fusion relevant conditions.

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