Atomistic Simulation of Neutron-Induced Radiation Damage in Fusion Reactor Materials Using Molecular Dynamics

Abstract

Future fusion reactors will operate under intense neutron irradiation, exposing reactor materials to extreme environments. High energy neutrons interacting with these materials generate energetic Primary Knock on Atoms (PKAs), which transfer their energy to surrounding lattice atoms and initiate collision cascades. These cascades produce a variety of irradiation-induced defects, including vacancies, self-interstitial atoms (SIAs), defect clusters, and dislocation loops. The accumulation and evolution of these defects significantly influence the micro-structural stability and mechanical properties of materials, leading to swelling, hardening, embrittlement, and ultimately limiting the service lifetime of fusion reactor components. Understanding of the mechanisms governing defect generation and evolution is essential for the development of materials for future fusion reactors. Molecular Dynamics (MD) simulations provide atomistic-level insight into collision cascade processes and serve as a complement to experimental irradiation studies.

This project aims to investigate neutron-induced radiation damage in selected materials using the open-source Molecular Dynamics package LAMMPS. Suitable interatomic potentials will be identified for fusion-relevant materials such as Steel, tungsten (W) etc. Atomistic models of these materials will be developed, and collision cascades initiated by PKAs with different kinetic energies will be simulated. The simulations will be used to quantify irradiation-induced defects, including vacancies, self-interstitial atoms, defect clusters, and their spatial distributions. Particular emphasis will be placed on understanding the influence of PKA energy on collision cascade evolution, defect production efficiency, and the number of surviving defects following cascade relaxation.

Note: The knowledge of crystal structure in materials is desirable. Students from chemical engineering may also apply.

Academic Project Requirements:

1) Required No. of student(s) for academic project: 1

2) Name of course with branch/discipline: M.E./M.Tech Material Science/Engineering

3) Academic Project duration:

(a) Total academic project duration: 32 Weeks
(b) Student's presence at IPR for academic project work: 3 Full working Days per week

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