Seminar

Institute for Plasma Research

Title : Molecular Dynamics study of defect diffusion

Speaker: Dr. Srinivasarao Bukkuru
Andhra University, Visakhapatnam

Date : 13th December 2019 (Friday)

Time : 03.30 PM

Venue : Seminar Hall, IPR

Abstract:

Primary radiation damage (PRD) in crystals refers to the process of energy and momentum transfer from an energetic projectile to the lattice atoms, causing atomic displacements in target material. The result of primary radiation damage event is creation of point defects (vacancies and interstitials) and their clusters. This primary radiation event lasts only about $10^{-11}s$. Subsequent events involve migration of the point defects and their clusters, recombinations to either nullify each other or forming precipitates and voids. These effects continue through out the operational lifetime of a reactor.

Comprehensive knowledge of primary radiation damage (PRD) and its effects is essential in developing new materials for advanced technologies such as semiconductor physics, nuclear power generation, etc. Radiation damage is a multi-scale phenomenon and it requires a multi-scale approach. Most of the existing experimental techniques do not have sufficient resolution to investigate these atomistic processes. There exist several simulation techniques that can provide better insights into these processes at different time and length scales. Molecular Dynamics (MD) and kinetic Monte Carlo (KMC) simulations are among them.

MD simulations have been carried out (i) to show how typically radiation damage can be quantified in terms of number of atomic displacements during the collision cascades (ii) to better identify the point defects created during the cascade events at different temperatures using “Max-Space Clustering (MSC)” method and (iii) to study the diffusion kinetics of both interstitials and vacancies in bcc Fe, Mo, Nb, W and fcc Ag, Cu, Ni, Pt single crystals.

The objectives of study are:

1. To better visualize and analyze the point defect configurations in collision cascades over a wide range of temperature without any assumed cut-off values.
2. To obtain temperature dependent cut-off values in a structured way instead of using assumed values for identifying the point defects.
3. To obtain better diffusion trajectories of point defects from MD simulations.
4. To estimate their diffusion parameters such as migration energies and preexponential factors of diffusion coefficients with better accuracy.
5. To quantify their correlational effects in terms of jump-correlation factor.
6. To study the diffusive-reactive-recombination reactions of these point defects.