Multi-scale Model of Material Damage due to Surrogate Ion Irradiation (SII)

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Energetic ions of several MeV are used to bombard materials in order to study the effect of neutron irradiation on materials – hence this is also called surrogate ion-irradiation. This is because the primary damage mechanisms in both cases are same and SII causes the same amount of displacement per atom (DPA) in a couple of days as neutron irradiation does in years, albiet in a smaller volume. The primary damage mechanisms like (i) collision cascades, (ii) in-cascade clustering to form sessile and glissile clusters, and (iii) diffusive recombination of defects, are at least qualitatively similar in both cases. Therefore SII is a useful method to gain an understanding of the mechanisms and to validate the codes and models used to simulate primary irradiation damage. A multi-scale model to simulate material damage due to SII is presented, which involves the following:

- A combination of Binary Collision Approximation Monte Carlo (BCA-MC) and Molecular Dynamics (MD) is used to obtain the primary damage state for several MeV proton irradiation of FeCr /Nb.

- Electronic stopping has been added in LAMMPS as a frictional force with the co-efficient of friction being obtained using the Lindhard-Scharff model [1].

- Machine learning is employed on a MD database to classify the in-cascade clusters based on shape, size and dimensionality. This is the first step to identify sessile and glissile clusters. With this the primary damage state of a material subjected to SII is obtained. [2]

- MD is used to obtain the diffusion parameters of interstitials and vacancies [3,4,5] and these parameters are passed to higher scale Kinetic Monte Carlo (KMC) simulations. Initial KMC results are discussed.

The talk aims to focus on the parameters that need to be passed across scales/models .

References:

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