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Statistical study of defects caused by primary knock-on atoms in fcc and bcc metals using molecular dynamics simulations

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Damage of materials due to neutron irradiation occurs via energetic cascades caused by energetic primary knock-on atoms (PKA) created by the energetic neutron as it passes through the material. These cascades result in creation of Frenkel Pairs (interstitials and vacancies). The interstitials and vacancies diffuse and recombine to (I) nullify the damage when an interstitial recombines with a vacancy, (II) form interstitial clusters when two or more interstitials recombine, and (III) form vacancy clusters when several vacancies come together. We report on molecular Dynamics (MD) simulations carried out in fcc (Cu) and bcc (FeCr) metals using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [1] to study:

1. Statistical variations in the number of Frenkel Pairs produced by energetic PKA directed in 1000 random directions. It is seen that at least 100 random directions have to be explored for the variance in the number of Frenkel pairs produced to become steady [2].
2. In-situ processing during MD simulations to find in-cascade cluster sizes and other parameters which are useful inputs for Kinetic Monte Carlo (KMC) / Dynamic Monte Carlo (DMC) studies. In-situ processing saves I/O of several tera-bytes when exploring 1000 random directions and shows no difference in run-time because the extra run-time processing is offset by the time saved in I/O.
3. Interstitialcy mechanism of interstitial diffusion, wherein an interstitial displaces a lattice atom thereby making the lattice atom an interstitial, in Cu, W and Fe. It is seen that the time-scale for *interstitialcy diffusion* is of the order of a few tens of pico-secs in these metals. This can contribute to further diffusive-recombinations of the Frenkel Pairs. Analysis of the diffusion process from a point of view of providing inputs to KMC/DMC will be discussed.

References

1. S. J. PLIMPTON, *Fast Parallel Algorithms for Short-Range Molecular Dynamics*, J. Comput. Phys., 117 (1995) 1; http://dx.doi.org/10.1006/jcph.1995.1039.
2. M. Warrier and M. C. Valsakumar, *Study of MD collision cascades in 1000 random directions in crystal Fe90Cr10 in the energy range 0.1 to 5 keV*, Fusion Science and Technology, 65, #2, (2014) 229-234.