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MOLECULAR DYNAMICS STUDY OF INTERSTITIAL DIFFUSION

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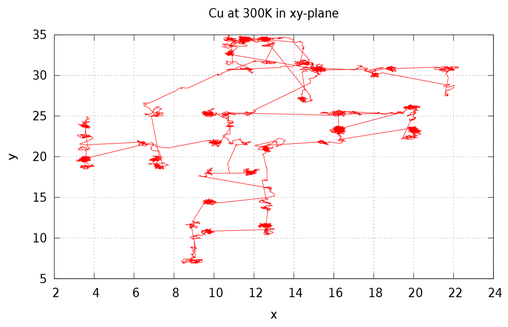
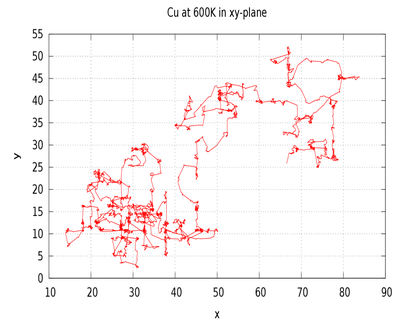
Motivation: To study the mechanism of interstitialcy diffusion in fcc and bcc single crystals at various length and time scales.

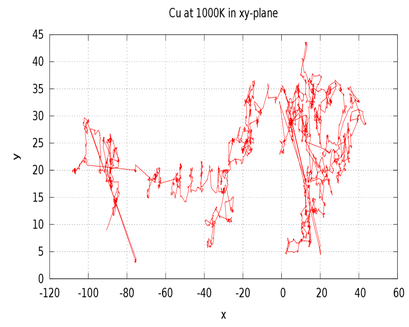
Introduction: Neutron irradiation of reactor materials creates energetic primary knock-on atoms (PKA) in the material, which cause collision cascades in the material resulting in Frenkel pairs. These Frenkel pairs can diffuse and recombine to neutralize each other and reduce damage, or form vacancies and interstitial clusters, thereby changing the material properties.

MD simulations: We carry out MD simulations to study interstitialcy diffusion in Cu, Fe and W. A cube of 10×10×10 unit cells is used. A single atom is introduced close to the center of the crystal and an NPT ensemble is used to equilibrate the system at 0 bar pressure. Periodic boundary conditions are used in all three directions with a time step of 1 fs. After equilibration, an NVE simulation is carried out to study the interstitial transport.

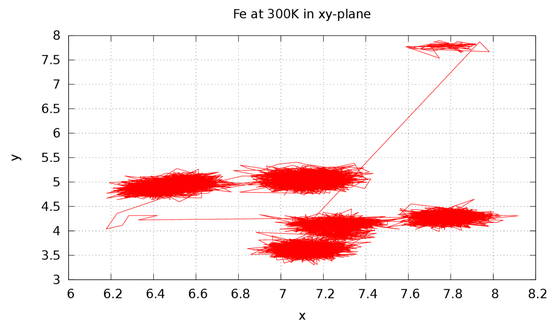
Interstitialcy Diffusion in Copper: For Cu, MD simulations were carried out in the temperature range 300K – 1200K. Both NPT and NVE simulations were carried out with a time step of 1fs.The NVE simulation was carried out for 360 pico seconds

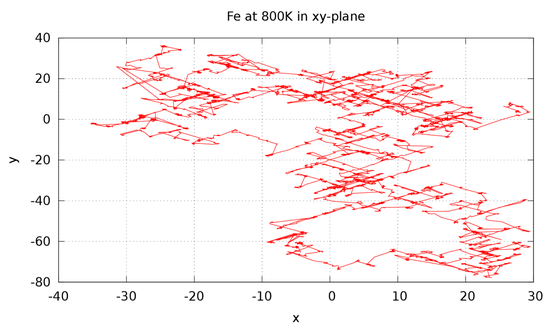


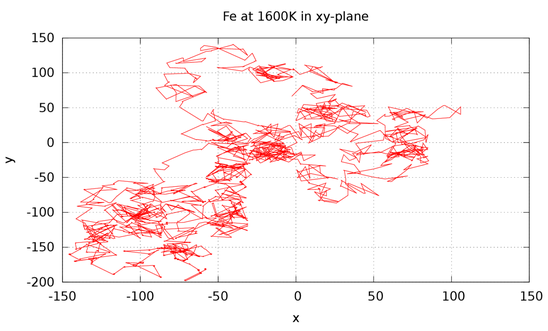




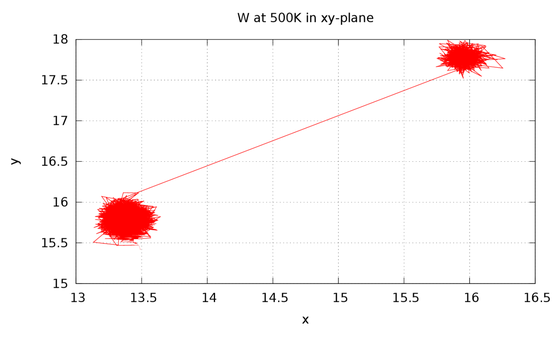
Interstitialcy Diffusion in Iron: For Fe, MD simulations were carried out in the temperature range 300K – 1800K. Both NPT and NVE simulations were carried out with a time step of 1fs.The NVE simulation was carried out for one nano second.

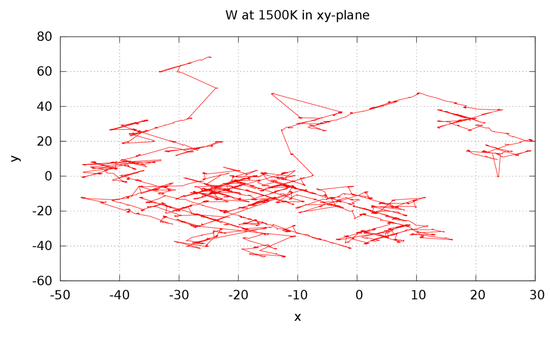


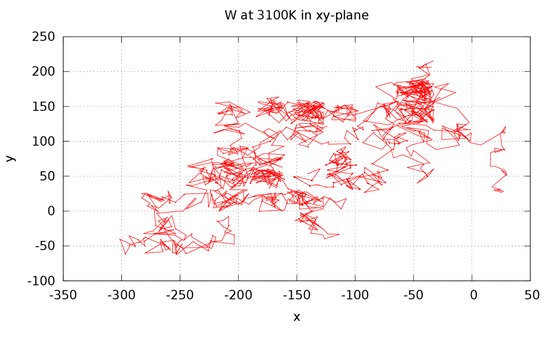




Interstitialcy Diffusion in Tungsten
For Fe, MD simulations were carried out in the temperature range 300K – 3500K. Both NPT and NVE simulations were carried out with a time step of 1fs.The NVE simulation was carried out for one nano second.

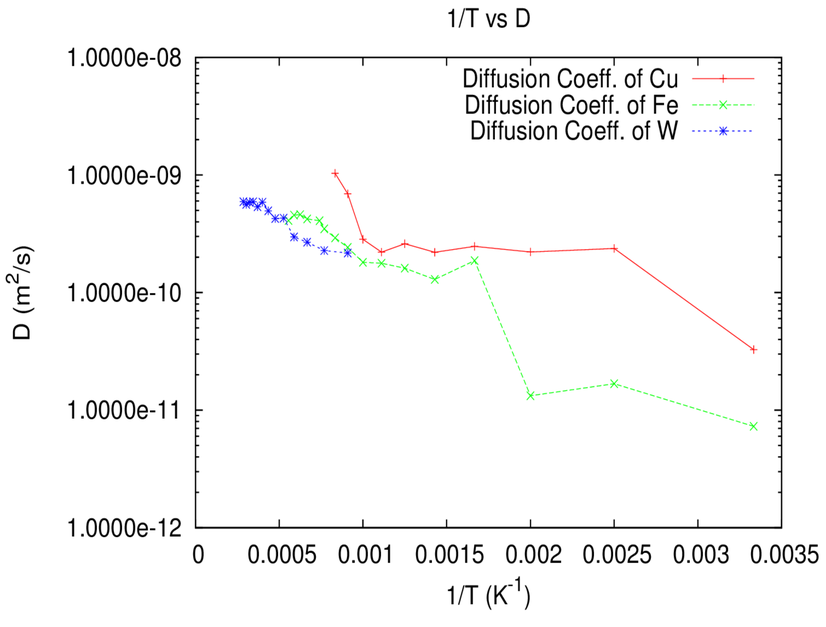






Results and Discussion

Interstitialcy diffusion, wherein an interstitial displaces a lattice atom and occupies its position, thereby making the lattice atom an interstitial, takes place in time scales of few tens of pico-seconds. Therefore this mechanism could be the dominant means of diffusion of interstitials post a collision cascade and could contribute to the formation of interstitial clusters, recombination, etc. We equate the MD trajectories to a random walk and calculate the interstitialcy diffusion coefficients. Longer MD simulations will be carried out to obtain the statistical errors in the random walk and do a proper Arrhenius like fit.



Acknowledgement:
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