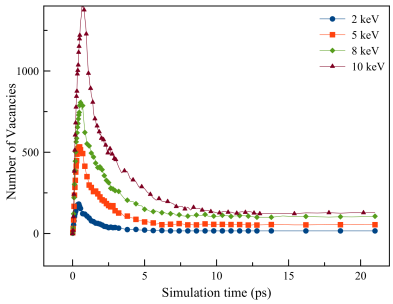
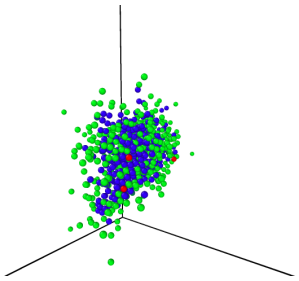
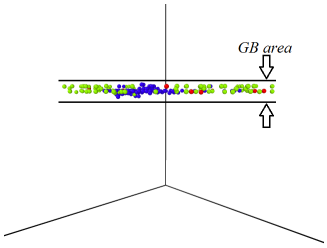
## Radiation damage of Fe-10%Cr

In this study, displacement cascades are generated in Fe-Cr structures of Cr concentrations between 2 and 10 at% by using primary knock-on atom (PKA) energies between 2-10 keV via molecular dynamics (MD) simulation technique. Single crystals (SC) and bi-crystal (BC) structures with three different [001] tilt grain boundaries (GBs) (e.g., **Σ**5 (310), **Σ** 13 (510), and **Σ** 17 (530)) have been simulated. The Wigner-Seitz cell criterion has been used to identify the point defects. The results show a marked difference between collisions observed in single crystals and those in bi-crystal structures. The Cr concentration does not seem to have any influence on the number of survived point defects. In bi-crystal models a large fraction of the total survived point defects (between 55 to 90%) tends to accumulate at the GBs, which seem to trap the generated point defects.

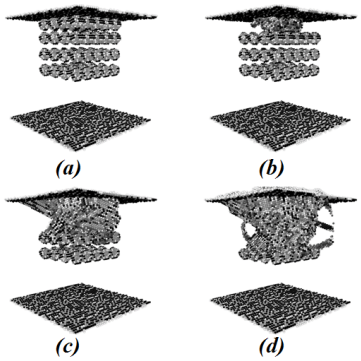


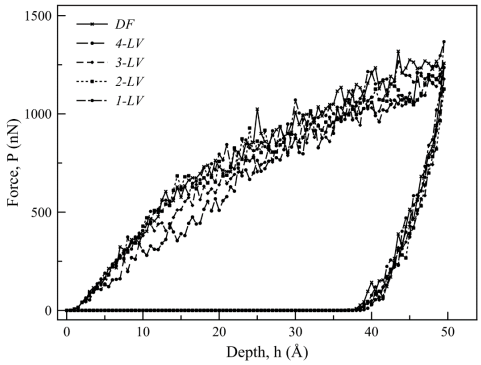






## Nanoindentation response of Fe-10%Cr with Voids

Nanoindentation response of single crystal Fe-10%Cr models has been performed using Molecular Dynamics (MD) simulation. Model of defects-free (DF) and models with voids of various sizes distributed over various spatial locations are researched. The load-displacement curve of the models with voids deviates from that of the DF model when dislocations start interacting with voids, which we call the “transition point (TP)”. The location of TP depends on the number of layers, size and position of the voids.



**Thermal conductivity of Fe-10%Cr with symmetric tilt boundaries**

The objective of this study is to examine the effects of grain boundary (GB)vdensity and temperature on lattice thermal conductivity (*k*) of Fe-10%Cr alloys containing different [001] tilt GBs. Three different [001] tilt boundaries (e.g. **Σ**5(310); **Σ**13(510), and **Σ** 7(530)) of various densities have been examined at sixteen different temperatures between 10K to 400K using the reverse non-equilibrium molecular dynamics (rNEMD) simulation technique. The results reveal GBs impose a resistance to the heat flow that causes a sharp temperature drop across the boundaries. Below 120K, the conductivity exhibits an inverse relationship with GB density, however above 120K the effect of GB density becomes insignificant. The variation of *k* with temperature shows three distinct regions: (i) between 10-90K, *k* decreases steadily with temperature; (ii) between 90-120K, a sudden drop in conductivity is observed; and (iii) above 120K, *k* becomes independent of temperature.