Materials Science and Technology Division
Materials Theory Group

"Modelling of Displacement Cascades in Thin Foils of Iron"

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Abstract

Recent molecular dynamic simulations of heavy-ion cascades in bulk iron have revealed a sub-picosecond shock-front mechanism for the creation of large interstitial clusters and that the nature of this final damage is determined early on before the thermal spike phase of the cascade.

A decelerating supersonic shock front produces a volume of destroyed lattice expanding away from the primary recoil event. Large self-interstitial clusters can be seen forming on the transonic boundary of this zone if it encounters for example a secondary cascade zone just ahead of this boundary. Where the two zones meet, the primary shock front injects atoms into the low-density core of the secondary event and a large interstitial loop is created and also enhanced vacancy loop formation at the cascade core.

Modelling has now been extended to include the effects of near-by free surfaces on self-ion cascades in iron. The interaction between the transonic shock boundary and the free surface soon after the pka event can greatly enhance the later vacancy dislocation loop production from self-ion cascades. Similar to the sub-picosecond interstitial capture mechanism by low density cores of secondary zones in the heavy-ion bulk study, the free surface can capture the higher density transonic boundary material, resulting in large groups of adatoms or if the cascades is sufficiently close to the surface, a crater with a rim of adatoms. Either way this leaves a high concentration of vacancies from the cascade core which later form 1/2[111] and [100] vacancy loops. Subsequent loss of 1/2[111] vacancy loops by glide to the free surface has also been directly observed.

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