Feb. 22th 2019

Effects of Solute-SIA Binding Energy on Defect Production Behaviors in Fe-based alloys

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Abstract

During primary damage, the fraction of produced solute interstitials in the total interstitials can be either higher or lower than the solute concentration in an alloy, depending on the solute type. To understand which alloy property governs the over- or under-production behaviors of solute interstitials, molecular dynamics simulations are conducted to simulate the cascade damage in a series of "artificial" Fe-Cr alloys with tunable binding energies between a substitutional solute (Cr) atom and a Fe self-interstitial atom (SIA). To achieve this, the Fe-Cr cross pair interaction in the interatomic potential is modified by multiplying a scaling factor so that the solute-SIA binding energy varies linearly from positive to negative values. It is found that the solute interstitial fraction has a strong correlation with the solute-SIA binding energy, and the correlation can be approximately described by a Fermi-Dirac-Distribution-like equation. The independent defect production results reported in literature are found to align well with this correlation. The correlation may be used to estimate the solute interstitial production behaviors in a wide range of Fe-based alloys simply based on the solute-SIA binding energy, without conducting laborious cascade simulations. It may also be used to improve the accuracy of predicting displacement per atom (dpa) of individual alloy constituents in the widely used SRIM software.

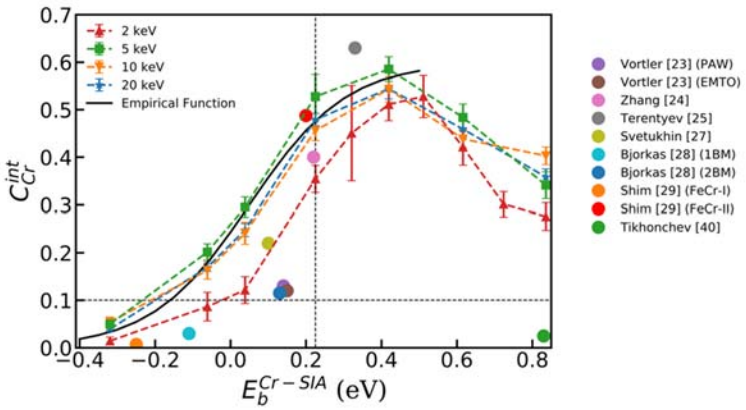

Fig. The fraction of solute (Cr) interstitials as a function of Cr-SIA binding energy for different PKA energies predicted by the modified potentials in a Fe-10%Cr alloy. The filled circles represent independent cascade simulation results reported in literature.

Biography

Yaxuan Zhang is a Ph.D. candidate advised by Dr. Xian-Ming Bai since July of 2016 and hopes to graduate in 2020. She received her bachelor degree in MSE department from Tianjin University, China, in 2015.