Reducing the uncertainty of the primary damage production in Fe

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One of the key questions for understanding neutron irradiation damage buildup in fission and fusion reactor steels is knowing the primary damage state produced by neutron-induced atomic recoils in Fe. Supporting this is our recent study revealing that the initial damage in Fe0.9Cr0.1 is essentially the same as in pure Fe [1]. In spite of decades of study, the question of what the amount and distribution of defects in Fe is, has remained highly unclear. Different computer simulations modules have given a good qualitative understanding of the cascade development [1,2]. However, quantitative differences of more than a factor of three have remained in the predicted clustered defect production numbers [2]. The disagreements between the potentials pose problems for finding a reliable predictive model for the behavior of Fe under irradiation.

In this study we analyze the initial damage as predicted by three recent interatomic potentials for Fe. These are well suited for a comparison because they have very different physical motivations and functional forms, but are comparable in overall quality and in particular reproduce the energetics of interstitials in different configurations well. The potentials are those by Ackland and Mendelev et al. (AMS) [3], the ‘magnetic’ potential by Dudarev and Derlet (DD) [4] and the Tersoff-like analytical potential by Müller, Erhart and Albe (MEA) [5]. The DD and MEA potentials were modified by us to describe high-energy repulsive interactions well. All potentials were then used in recoil collision cascade simulations carried out and analyzed in exactly the same manner for all potentials.

Analysis of the resulting damage showed a much smaller uncertainty regarding the damage production than that of previous potentials. The total defect production numbers essentially agree within the statistical uncertainty for the three potentials. Some differences remains regarding the defect clustered fractions, but these are clearly smaller than the variations between previous potentials. The remaining differences between the fractions are ascribed to the different descriptions of the melting point and of the interstitial mobility in the potentials, and may be so small that they would not have consequences for the later stages of damage evolution.


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