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Effects of the short-range repulsive potential on cascade damage in iron

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Abstract

Recent work has shown that the repulsive part of the interatomic potential at intermediate atomic separations strongly affects the extent and morphology of the damage produced by collision cascades in molecular dynamics simulations. Here, we modify an existing embedded atom method interatomic potential for iron to more accurately reproduce the threshold displacement energy surface as well as the many-body repulsion at intermediate and short interatomic distances. Using the modified potential, we explore the effects of an improved repulsive potential on the primary damage production and the cumulative damage accumulation in iron. We find that the extent of the damage produced by single cascades, in terms of surviving Frenkel pairs, directly correlates with the change in threshold displacement energies. On the other hand, the damage evolution at higher doses is more dependent on the formation and stability of different defect clusters, defined by the near-equilibrium part of the interatomic potential.

Keywords:
interatomic potential, threshold displacement energy, molecular dynamics, iron, collision cascade

1. Introduction

Atomistic simulations have during the last decades been a widely used tool for studying radiation damage production on the atomic level. In metals, the development of accurate embedded atom method (EAM) [1] interatomic potentials has opened the possibility to extract more and more quantitative information from atomistic simulations. EAM potentials rely on the principles of density functional theory, and have been successful in describing near-equilibrium properties of metals and metal alloys [2, 3]. However, when modelling radiation damage, the atomic system is pushed far from its equilibrium crystalline state, which consequently sets high demands on the interatomic potential.

Interatomic potentials for radiation damage studies require not only a good description of the equilibrium properties, but also a realistic description of short-range forces experienced as atoms with high velocities move through the lattice. Ziegler et al. have showed that the repulsive potential for any atom pair can be fairly accurately described by a universal potential in the form of a screened Coulomb potential [4]. When developing interatomic potentials applicable for radiation damage simulations, it has long been a standard approach to let this universal ZBL potential describe the repulsive interactions at short interatomic distances (below around 1 Å) [5–7]. However, the ZBL potential must be smoothly connected to the given near-equilibrium potential, be it an EAM potential, a Tersoff potential [8] or any other many-body potential. The transition between the ZBL and the equilibrium potential is typically achieved by a simple function defining the intermediate repulsive range [6]. This intermediate range can be tuned to reproduce the correct threshold displacement energies (TDEs). The combined potential then makes it possible to accurately model both highly repulsive forces and near-equilibrium properties, both which are important when simulating the evolution of a radiation damage event in a material. However, recent work [7, 9] has shown that using the TDEs as the only criterion when fitting the intermediate transition part can still result in widely different potentials with large differences in radiation damage results. More emphasis should therefore be put on fitting the transition range.

Recently, radiation damage modelling has also focused on the damage produced by cascades overlapping with pre-existing damage, and the evolution of the defect structures at higher damage doses [10–13]. The rate of damage accumulation and clustering of point defects in overlapping cascades is dependent on the repulsive part of the potential. Furthermore, the types of defect clusters produced at higher doses, and their stability and evolution after subsequent collision cascades, is dependent on the energetics of the defect clusters given by the interatomic potential. However, little attention has been paid to the resulting differences in the higher-dose cascade damage due to differences in the interatomic potential.

In this work, we adjust an existing EAM potential for iron [14, 15] to more accurately reproduce experimental and *ab initio* data sensitive to the intermediate repulsive

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