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Molecular dynamics simulations of threshold displacement energies in Fe

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Abstract

We compare systematically the threshold displacement energy surface of 11 interatomic potentials in Fe. We discuss in detail different possible definitions of threshold displacement energies, and how they relate to different kinds of experimental threshold displacement energies. We compare the threshold results to experiments, and find that none of the 11 tested potentials agrees fully with experiments. However, all the potentials predict some qualitative features in the same way, most importantly that the threshold energy surface close to the 1 0 0 crystal direction is flat and that the largest threshold energies occur around very roughly the 1 2 3 crystal direction.

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1. Introduction

One of the basic quantities defining the radiation resistance of a material is the threshold displacement energy, i.e. the energy needed to displace an atom in a material to create a stable Frenkel pair. The concept of threshold displacement energy was probably devised by Wigner in the early 1940s, as reported by Burton [1], and already in 1949 it appeared as a functional parameter in Seitz's model to treat elastic collisions [2], where it was assessed as equal to the sum of the cohesive energy plus the formation energy of the Frenkel pair (in total about 25 eV). Since then it has played a key role in radiation damage theory. For example, if the amount of radiation-induced defects increases linearly with energy, the damage level can be well predicted by the Kinchin–Pease (or its variation NRT [3]) equation which states that the amount of damage is proportional to the ratio of the nuclear deposited energy and an effective threshold displacement energy E_d^* [4]. Even in materials where the Kinchin–Pease equation is not valid, typically dense metals, the damage level is often given in terms of a cascade efficiency which is the actual number of defects compared to the Kinchin–Pease prediction [5,6]. Because of this, it is of importance to know the value of the threshold displacement energy in any material where irradiation effects are of interest.

The threshold displacement energy has been studied both experimentally and by computer simulations in a wide range of materials (see e.g. [7–10] and references therein). From an application point of view, of particular interest is the threshold displacement energy in Fe. Radiation damage in Fe-based materials is of great interest because the main structural materials in fission and fusion reactors are steels. In addition, it is possible to use ion implantation to harden steels. Thus it is surprising that the threshold

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displacement energy in Fe has in fact been studied less than in many other materials. The average threshold displacement energy most frequently used for Fe, the so-called NRT or ASTM standard, is 40 eV [11]. Its source in literature review papers [7,8] is often cited to be [10], but this paper is also a review and bases its value on the MD simulations carried out by Erginsoy et al. in 1964 [12]. There is one experiment by Lucasson which gives an average threshold energy of 24 eV for Fe [13], but in his later review papers even Lucasson himself does not use this value [10], apparently because the result is dependent on the choice of the damage model. The experiments which do exist give only the threshold energy along the low-index lattice directions 100 [14], 110 and 111 [15,16], not the average over all directions, that would be most appropriate for the effective threshold displacement energy used in the Kinchin–Pease formulation.

There have been significant advances in not only computer capacity but also in the understanding of interatomic interactions since 1964 [17–19], including additional theoretical works on the threshold displacement energy in Fe. Agranovich and Kirsanov [20] studied the threshold energies close to 100 and 111 including thermal displacements (in contrast to the work of Erginsoy et al. that was carried out at 0 K) and obtained threshold energies of 18 eV around 100 and 26 eV around 111, in fairly good agreement with the experiments of Lomer and Pepper [15]. Apparently the first systematic simulations of threshold energies in Fe employing many-body potentials were carried out by Bacon et al. [21] who in 1993 simulated threshold energies with the Finnis–Sinclair potential [17], modified in the repulsive part [22]. They obtained thresholds of 18 eV around 100, 30 eV around 110 and >70 eV around 111 at 0 K. Soon after this, Doan and Vascon [23] adjusted another Fe potential [24] with a repulsive potential in a manner which gave good agreement with experiments [23]: 21 eV around 100, 31 eV around 110 and 18.5 eV around 111. Also several other, less detailed, studies of the threshold displacement energies have been carried out in the context of adjusting the repulsive part of the potentials to have a realistic high-energy part (see Section 2.3). However, none of the works on the threshold energy in Fe have affected the NRT standard. Moreover, the works have used slightly different (and sometimes poorly documented) definitions of what the threshold energy is, especially regarding whether it is calculated in the exact crystallographic direction, or in some angular interval around it to account for electron beam spreading. Hence it is of interest to review the threshold energies given by different models using the same threshold energy definitions for all the potentials.

In the current paper we systematically reexamine the issue of the threshold displacement energy in Fe. We simulate the full three-dimensional threshold energy surface using 11 different interatomic potentials, taking care that all non-physical simulation parameters (such as the simulation cell size) are chosen so that they do not affect the end result. We compare the results of all potentials with each other and experiment. We also discuss the original simulations by Erginsoy et al. in view of the present simulations.

2. Method

2.1. Definition of threshold displacement energy

It might seem to be straightforward to define a threshold displacement energy of a material. However, one can in fact define several different threshold displacement energies depending on the viewpoint and the experimental situation one wishes to model. Since distinguishing between these is important for understanding some of the results of this paper, we review here different possible definitions.

The most straightforward distinction comes from consideration of irradiation geometry. First of all, it is possible to define a direction-specific threshold for each lattice direction, $E_d(\theta,\phi)$. This can be measured by electron irradiation of a thin single crystal specimen [25]. The full function $E_d(\theta,\phi)$ forms the threshold energy surface. An average threshold energy E_d^{ave} can be defined as the average of the function $E_d(\theta,\phi)$ over all angles.

However, this picture is not the end of the story. Because of thermal and zero-point lattice vibrations [26] atoms never reside exactly on perfect lattice sites. Hence even for the exact same lattice direction, it is possible that a given energy sometimes produces a defect, sometimes not. This lead Malerba and Perlado to introduce the concept of lower and upper thresholds, lower (E_d^l) being the value where a defect sometimes is produced, upper (E_d^u) being the one where it is always produced [27]. This definition was useful in their study of SiC, but the quantity E_d^u is problematic in metals where in-cascade annealing can cause all damage to recombine with a non-zero probability even for very high energies. This non-monotonousness of the threshold displacement energy is illustrated in Fig. 1, which shows the probabilities to form at least one defect $P_{def}^i(E)$ for individual directions i. Note that in one of the cases there is sometimes no damage produced even at an energy of almost 600 eV. Animation of these cases showed that this is a dynamic annealing effect, where an interstitial is formed for a short time, but recombines with the vacancy left at the original site of the recoil before the cell has cooled down. From simulations of defect production with all 11 potentials up to 250 eV we found that for a given direction the probability of a uniform defect production curve (i.e. where a defect is always produced above the lower threshold) is in fact only 10%.

Although one could argue that it is the lower threshold which is the true threshold, the realization of the possibility of recombination at high energies has consequences on the definition of the average threshold displacement energy. Namely, one can choose to either take into account or not take into account the events above E_d^l in the calculation of the average threshold energy. That is, if one uses the