TEMPERATURE DEPENDENCE OF DEFECT PRODUCTION EFFICIENCY IN α-FE

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Abstract

Advanced high-strength steels are being considered for various next generation nuclear reactor components due to their relatively good neutron transparency and thermo-mechanical stability. In the current study, we generate comprehensive displacement cascade defect statistics for α-Fe by considering temperatures between 15 and 1200 K, PKA energies between 0.1 and 20 keV and three interatomic potentials. The data is analyzed in terms of the defect production efficiency η, which is a measure of the severity of primary displacement cascade damage and is defined, from molecular dynamics simulations, as the number of surviving Frenkel pairs observed from simulation relative to the number of stable Frenkel pairs predicted from the Norgett-Robinson-Torrens (NRT) model. Previous studies have revealed that η is independent of interatomic potential and temperature and exhibits power-law dependence with PKA energy. Our results contrast with previous studies, as η is shown to be temperature dependent. This temperature dependence can be attributed to defect recombination, which is a thermally activated mechanism. Based on our findings, we propose an extended power-law representation for η, which accounts for the influence of both temperature and PKA energy.

1. Introduction

Next generation nuclear reactors require extensive materials selection, development and performance evaluation as material degradation may potentially limit the successful implementation of the various reactor designs being considered. In particular, materials used in the reactor core must be able to withstand more severe radiation dosages, temperatures and pressures as compared to current reactors [1-5]. Advanced steels are being considered as a candidate material for next generation nuclear reactors due to their relatively good neutron transparency and mechanical stability at high temperature and pressure [6]. However, steels are generally susceptible to radiation damage in the form of radiation-induced embrittlement and irradiation creep [7, 8].

The underlying mechanism of the radiation damage lies in the evolution of defects induced by the displacement cascade. Neutron incited displacement cascades produce an excess concentration of vacancies and self-interstitial atoms (SIA), driving microstructure evolution and ultimately affecting macroscopic thermo-mechanical properties. Hence, understanding displacement cascade is important for the nuclear industry. Experimental studies are required to assess and understand radiation damage, nevertheless, such studies are expensive due to the inherent difficulty of handling irradiated materials and the wide range of time and length scales involved. In this regards, molecular dynamics (MD) simulations are ideally suited for computational study of various aspects of radiation-induced damage.

A standard method to assess the severity of displacement cascade damage is to determine the efficiency of defect production for a given neutron collision. This is done by determining the parameter η, the defect production efficiency. In MD simulations, η is found by scaling the number n^{MD} of surviving Frenkel pairs (FP) observed from the computations, with the number n^{NRT} of stable FP predicted from the Norgett-Robinson-Torrens (NRT) [9, 10] model and is given by,

$$\eta = \frac{n^{MD}}{n^{NRT}} = \frac{n^{MD}}{0.4}\frac{E_d}{E_p} \tag{1}$$

where E_d is an average threshold displacement energy [11], which is assumed to be temperature and neutron energy independent, and E_p is the energy transferred to the PKA due to the incident collision. The NRT model is a modified form of the Kinchin-Pease model [12], which assumes a sequence of binary atomic collisions and therefore neglects many body effects. Following standard practice, E_d for α-Fe is taken equal to 40 eV [9, 13-15].

Molecular dynamics displacement cascade damage studies on α-Fe have focused on the influence of PKA energy with temperature [15-20], interatomic potential [13, 14, 21-23] and solute additions for alloys such as Fe-Cr [24-27], Fe-He [28, 29], Fe-Ni [30, 31] and Fe-P [32] on defect statistics and clustering. A recent critical review [13] of the displacement cascade literature for α-Fe has found that η is independent of temperature and interatomic potential, at least for interatomic potentials that correctly reproduce relevant irradiation defect energies. The general trend observed is that η decays in an approximately exponential manner with PKA energy from an average value of 1.22 at 0.1 keV to a plateau value of 0.30 at 5.0 keV. The spread in η is noticeably higher at lower PKA energies as compared to the plateau region. For example, Malerba's compilation [13] shows that η is 0.44 at 0.1 keV and converges to approximately 0.12 at 5.0 keV. Bacon et al. [17] were the first to find that the decay in η with PKA energy can be described by a power-law relationship of the form,

$$\tilde{\eta} = 0.1A(E_p)^{m-1} \tag{2}$$

where the prefactor A and exponent m are empirical constants. The values of A and m are reported to be temperature independent. Previous studies [15, 17, 24] have reported A values between 4.2 and 5.70 and m values between 0.78 and 0.80 for α-Fe.

Our objective in the current study is to generate a consistent set of primary displacement cascade defect statistics for α-Fe by considering a wide range of temperatures and PKA energies relevant to next generation nuclear reactors for various interatomic potentials. We pay particular attention to the influence of defect identification method on defect statistics, and in doing so develop a new method based on a temperature dependent search radius.

2. Simulation Technique

Displacement cascade simulations on α-Fe were performed using LAMMPS, a molecular dynamics code distributed by Sandia National Laboratories [33, 34]. A wide range of simulation conditions are considered: the simulation matrix consists of five temperatures (15, 300, 600, 900 and 1200 K), seven PKA energies (0.1, 0.5, 1, 5, 10, 15 and 20 keV) and three interatomic potentials, denoted as ABC [35], AMS [36] and DDNB [22, 37] in the current work.

The ABC [35] interatomic potential is of Finnis-Sinclair type and is fit to ab-initio data to accurately describe bulk properties. This potential does not produce reliable defect energies [14]. However, the ABC [35] potential and earlier versions have been much used for displacement cascade studies [14, 16, 19] and is therefore used for comparison with results from the more recent interatomic potentials. The AMS [36] interatomic potential is an embedded-atom method (EAM) interatomic potential and is fit to ab-initio values of both bulk properties and point defect formation energies. In particular, this potential provides a more accurate description of dumbbell defects. The DDNB [37] many-body empirical potential, originally formulated to treat the effect of magnetism on the energy of interacting Fe atoms, was modified by Björkas and Nordlund [22] for use in displacement cascade simulations. Similar to the AMS potential, it leads to acceptable reproduction of defect formation energies.

The simulation cell was built such that the crystal lattice was oriented with the < 100 > crystal axes parallel to the external x, y and z directions. Periodic boundary conditions were used. The appropriate simulation cell size was determined based on PKA energy with the total number of atoms ranging from 65536 to 877952. Prior to conducting the cascade simulations, the energy of the crystal was minimized using a conjugate gradient scheme. The simulation cell was then relaxed using an isothermal-isobaric ensemble (constant NPT integration) at the temperature of interest and with pressure equilibrated to zero.

Displacement cascades simulations were studied using the statistics of the microcanonical ensemble (NVE). Displacement cascades were initiated in the equilibrated cell by imparting a kinetic energy to a primary knock-on-atom (PKA) along the < 135 > crystallographic direction. This high index direction was chosen to avoid channelling [16] and to simulate representative cascade behaviour [38]. In order to obtain better defect statistics, five simulations were performed at each condition by choosing distinct < 135 > PKA directions. Furthermore, a variable time-step was adopted for cascade simulations to improve numerical stability and computational efficiency.

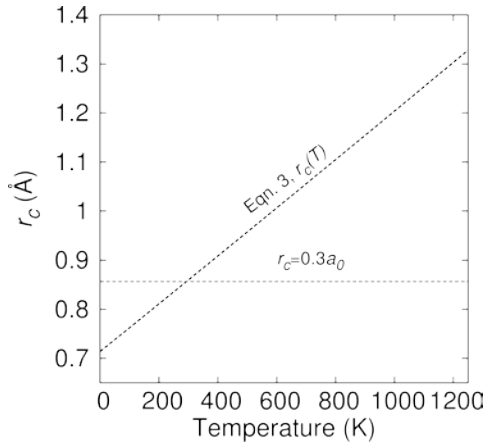


Figure 1 Variation of defect identification search radius as a function of temperature compared to constant search radius of $0.30a_o$.

Radiation-induced point defects are most often identified in molecular dynamics simulations using either a constant search radius, which emanates from the lattice sites, or by associating each atom

with its nearest lattice site. The latter method is often called the Wigner-Seitz defect identification method. A commonly used approach for the former method is to select r_c approximately equal to $0.30a_o$ [14, 16, 39]. In the current work, we develop an equation for a temperature dependent search radius for identifying point defects. Our equation is based on a statistical analysis of atom position with temperature. Lattice thermal expansion is also considered. The temperature dependent search radius $r_c(T)$ is given by,

$$r_c(T) = (r_0/a_0 + \beta T)\, a_T \tag{3}$$

where a_o and a_T are the lattice constants at 0 K and temperature T respectively, r_o is the search radius at 0 K, β is the rate of change of the dimensionless search radius with temperature and $a_T = a_o$ [1 + $\alpha_T T$], where α_T is the co-efficient of linear thermal expansion. The results of our statistical analysis are shown in Figure 1. We compare $r_c(T)$ versus $r_c = 0.30a_o$ where the parameters a_o = 2.86 Å, $\alpha_T = 11.76 \times 10^{-6}$ K^{-1} [40], $r_o = 0.25a_o$ and $\beta = 1.67 \times 10^{-4}$ K^{-1} have been used. We find that $r_c(T)$ varies approximately linearly from 0 K to 1200 K.

3. Results and Discussion

Defect production efficiency η has been calculated using Eq. (1) for the three interatomic potentials used in the current study. The results are plotted versus PKA energy in Figure 2. Similar trends are observed for all interatomic potentials studied; η decays in an approximately exponential manner with increasing PKA energy and reaches a plateau at approximately 5 keV. However, the rate of decay with PKA energy and the plateau values obtained depend on temperature.

We find that our η values follow a distinct trend and shift downward in an orderly fashion with increasing temperature. The variation of η with temperature for a given PKA energy is higher at lower PKA energies. For example, considering all interatomic potentials used, Figure 2 shows that η varies from 2.20 to 0.70 at 0.1 keV and from 0.75 to 0.20 at 10 keV over the temperature range considered. The η values generated in our study are compared with the data compiled in Malerba's critical review [13], as shown by the grey regions in Figure 2. This compiled data set includes η values from previous studies generated using various interatomic potentials, temperatures and defect identification methods. The general trend of decay with PKA energy exhibited by our data agrees with that of the compiled data, however, unlike our data the compiled data does not show a noticeable temperature dependence. Furthermore, our low temperature data, 300 K and below, generally lies above the compiled data set. One reason for this difference is that at temperatures less than 300 K we are using a more stringent search radius (see Figure 1) and therefore expect to detect more defects. Another reason is that the compiled data uses a variety of defect identification methods, including the Wigner-Seitz method. The Wigner-Seitz method can significantly under-predict primary cascade defect numbers when dumbbells are a significant fraction of the defect population and in clusters, which is the case for α-Fe. This error arises as clustered dumbbells often share a common SIA, which will not be properly accounted for by the Wigner-Seitz method.

An analysis of our generated defect statistics show that the power law relation of Eq. (2) can be modified in a relatively simple manner to include the influence of temperature. We propose a decay function for prefactor A such that,

$$A = c_s + (c_o - c_s)\,\mathrm{sech}(b\,T/T_m) \tag{4}$$

where T is the simulation temperature, T_m is the melting temperature and is taken to be 1820 K for Fe, and c_o, c_s and b are empirical constants. For each temperature studied, A and m are obtained from a log-log plot of η versus PKA energy, i.e. from the data presented in Figure 2. Exponent m is found to be approximately constant with temperature and falls between 0.70 and 0.84 for the interatomic potentials considered (Figure 3(a)). The average value obtained considering all temperatures studied is m=0.77, which is in agreement with other studies [15, 17, 24]. Prefactor A decreases significantly with temperature (Figure 3(b)), from an average value of 12.6 at 0 K to 4.0 at 1200 K. The empirical constants, thus obtained by fitting Eq. (4) to the data in Figure 3(b), are given as c_o=12.6, c_s=4.0 and b=6.0. Equation (4), plotted using the derived constants, leads to an acceptable description of the temperature dependence of prefactor A as shown in Figure 3(b).

Although previous studies have generally concluded that the influence of temperature on η is negligible, a re-examination of those studies [15, 17, 18, 20, 41] which did consider a wide range of temperatures reveals a small yet consistent temperature dependence to η. Similar to the description of our data, η is found to decrease with increasing temperature, where the difference in η with temperature is larger at small PKA energies. For example, the results presented by Bacon and co-workers [16, 17] on η for α-Fe show that when temperature is increased from 100 to 600 K at a PKA energy of 0.5 keV η decreases by 0.30, whereas the same temperature increase at higher PKA energies leads to a decrease in η of 0.06. Similar observations have been made by Gao et al. [18], who report a drop in η of 0.18 at 2.0 keV and 0.08 at 5.0 keV when temperature is increased from 100 to 900 K. Stoller's [15, 20] investigations on defect production efficiency of α-Fe shows that η decreases by 0.07, from approximately 0.34 at 100 K to 0.27 at 900 K, for PKA energies of 10 keV. These trends are consistent, yet the temperature dependence of η is smaller in magnitude, as compared to our results.

The discrepancy between our results and previous studies can be attributed to our use of Eq. (3) for primary cascade defect identification, as opposed to the use of either constant search radius or Wigner-Seitz methods. Modification to the defect identification procedure was necessary to analyse defect statistics generated over a wide range of temperatures and to accurately account for dumbbell defects, whose formation energies relative to other radiation-induced defects possibly change with temperature. Justification for the new defect identification method lies in the need to account for thermal lattice expansion and the influence of kinetic energy on atom position when considering a wide temperature range. Furthermore, our study is the first data set to address a comprehensive matrix of PKA energies and temperatures relevant to next generation reactors, such as the Supercritical-Water-Cooled Reactor (SCWR), whilst using consistent analysis methods. Although the number of defects during the thermal spike phase increases with increasing temperature [16, 18, 42], we speculate that an increase in recombination efficiency leads to a lower observed n^{MD} and hence a lower η with increasing temperature.

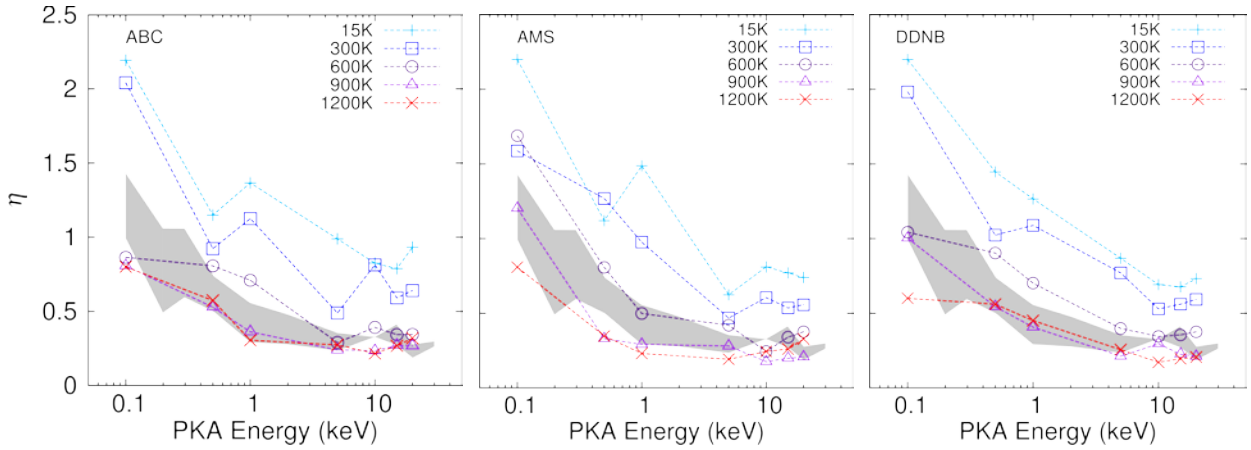
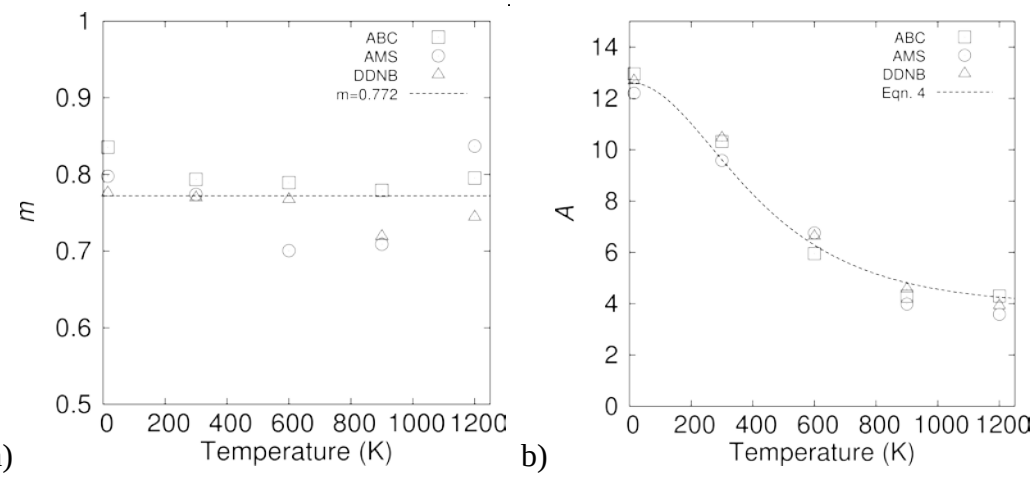


Figure 2 Defect production efficiency versus PKA energy for the ABC, AMS and DDNB interatomic potentials. The results are compared to compiled data (grey shaded area) as shown in Figure 1 from Malerba's critical review [13]. Note that the outlying data as shown in Figure 1 [13] were deemed unacceptable by Malerba and are not reproduced in our figure.



a) b)

Figure 3 a) *m* and b) *A* versus temperature for the interatomic potentials studied. The line in a) represents the value of m averaged over interatomic potential and temperature and b) represents the best fit curve following Eq. (4).

4. Conclusion

Comprehensive displacement cascade defect statistics were generated for α-Fe over a wide range of PKA energies and temperatures. The primary displacement cascade defects are analysed in terms of defect production efficiency η. Although previous studies have shown that η is independent of temperature, our results show η to be temperature dependent. This temperature dependence can be attributed to defect recombination, which is a thermally activated mechanism. Based on our findings, we propose an extended power-law representation for η, which accounts for the influence of both temperature and PKA energy.

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