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The effect of temperature on primary defect formation in Ni–Fe alloy

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ABSTRACT

Molecular dynamics (MD) simulations have been used to study the influence of temperature on defect generation and evolution in nickel and Ni–Fe alloy (with 15% and 50% Fe content) with a 10-keV primary knock-on atom (PKA) at six different temperatures from 0 to 1500 K. The recently available Ni–Fe potential is used with its repulsive part modified by Vörtler. The temporal evolution and temperature dependence of stable defect formation and in-cascade clustering processes are analysed. The number of stable defect and the interstitial clustering fraction are found to increase with temperature whereas the vacancy clustering fraction decreases with temperature. The alloy composition dependence of the stable defect number is also found for the PKA energy considered here. Additionally, a study of the temperature influence on the cluster size distribution is performed, revealing a systematic change in the cluster size distributions, with higher temperature cascades producing larger interstitial clusters.

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1. Introduction

High-performance alloys will be critical for the success of future fission and fusion reactors. They are required to maintain their structural integrity when exposed to unprecedented fluxes of high-energy neutrons and intense thermomechanical stresses [1,2]. Under such conditions, alloys can degenerate and lose their function because of the aggregation of point defects produced by irradiation. The point defects aggregate to form various types of defect structures, leading to swelling, hardening, and embrittlement or amorphisation of materials [3,4]. This will affect the lifetime and safety of the reactors.

A huge amount of experimental and theoretical efforts have been put forth to model the undesirable irradiation effects on the mechanical properties in future fission and fusion reactor materials, with significant attention being paid to displacement cascades [5–10]. It is not currently possible to directly observe the behaviour of displacement cascades because of their short time scale and small volume, so the method of molecular dynamics (MD), whose length and time scales are compatible with displacement cascades, has been broadly applied to understand primary radiation damage formation. These studies have established several consistent trends in primary damage formation in a number of materials [11]. The number of Frenkel pairs, N_f, has been shown to follow a power-law dependence on the cascade energy over a broad energy range, and the ratio of MD stable displacements divided by the number obtained from the NRT model [12] decreases with energy until subcascade formation becomes prominent. The cluster behaviour (the clustered fraction of SIAs and the structure of the cluster formed) still remain rather unclear because it depends on many factors, including crystal lattice structure, stacking fault energy, the energy of the primary knock-on atom, E_{PKA}, and irradiation temperature [13–16]. Irradiation temperature has a significant effect on the evolution of radiation damage in metals because the motion of defects and the dissociation of their clusters are thermally activated processes [14]. The effect of irradiation temperature on iron, copper, and plutonium alloy has been reported in numerous studies [17–20]; however, these previous studies cover either a limited temperature range or low primary knock-on atom (PKA) energy. Hence, more theoretical data are needed to give a reliable description of the thermal effect on irradiation.

Except for simulations of displacement cascades for pure elements, binary alloys are usually used as a surrogate system for a complex actual alloy, because modelling such a complex system on the atomistic scale is not practical at this time [6,7,9,11,10]. In previous studies, particular attention has been paid to austenitic and ferritic–martensitic steels, primarily because of the likely use of low-activation ferritic steels in future fission and fusion reactions. Ni-base alloy—for example, the austenitic matrix Ni–Fe alloy, which has also been considered to be a promising candidate material for future fission and fusion reactors—has not been extensively studied on the atomistic scale. One reason for this is that its potential for describing the ferritic and austenitic phase stability has only recently become available [21]. Furthermore, the repulsive part, which describes very short ranged interactions in radiation damage simulations, has recently been adapted for cascade

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simulations [10]. The previous study on Ni–Fe alloy focussed on the effect of prolonged irradiation [10] and, as far as we know, information on the thermal effect is still limited. Therefore, a systematic study of the effect of temperature on the primary damage of Ni–Fe alloy is warranted to understand the material behaviour under the extreme conditions of a nuclear reactor.

The goal of the present work is to use molecular dynamics simulations to describe the temperature dependence of Fe–Ni alloy primary radiation damage formation for which the data are limited. The simulation and identification techniques are summarised in Section 2. The simulation results and our discussion are presented in Section 3. Concluding remarks are given in Section 4.

2. Simulation method

All simulations here were performed using the MD code LAMMPS [22]. The production of a cascade was initiated by the energetic recoil PKA (a chosen Ni atom at the top centre of the simulation cell) and the subsequent displacement cascades, recombination, and in-cascade clustering of point defects were simulated in full detail. In our simulations, we used a cubic MD block of 500 000 atoms for 10-keV cascades The block is much larger than the empirical block size usually used to avoid overlap of the cascade with itself by virtue of the periodicity.

After being given the initial lattice temperature, the block was equilibrated for several picoseconds before the PKA event was initiated to ensure that the lattice thermal vibrations (phonon waves) were established for the simulated temperature. Each cascade corresponded to a different PKA position. To each side of the block, we applied a one-cell-thick Langevin thermostat to avoid the average temperature rise caused by the distribution of the PKA's kinetic energy. Subsequently, we chose a Ni atom from the top middle of the simulation cell and gave the atom 10 keV of kinetic energy in the form of an instantaneous velocity. For all simulations, a high-index direction [135] was used for the PKA to minimise directional effects such as channelling and directions with particularly low or high displacement thresholds. To obtain a small standard error about the mean number of defects produced, we performed 10 simulations for each simulated condition.

MD simulation results depend on the interatomic potential. In this work, the original equilibrium potentials for the Fe–Ni system [21] are used. These include our own Fe–Ni embedded atom method pair potential and the transformed original Ni and Fe potentials [23,24]. The original Fe–Fe potential already includes a well-tested repulsive part, and the repulsive interactions of Ni–Ni and Fe–Ni have recently been modified by Vörtler [10] using Ziegler–Biersack–Littmark (ZBL) repulsive potentials [25].

The final atomic configuration was evaluated on the basis of the Wigner–Seitz (W–S) cell method and the point defects were defined according to the number of atoms from the output geometry found in each reference cell. Interstitial clusters were defined by a third-nearest-neighbour (NN) criterion, as used in [8]. Since the in-cascade vacancy clustering in iron was quite low, we used the fourth-NN criterion, for which peaks in the distributions of vacancy–vacancy separation distances were obtained.

3. Results and discussion

3.1. Point defect number

Next, we examined the number of Frenkel defects through simulated time and temperature. We first studied the average peak value of the defect numbers at each temperature. Although the average peak value fluctuates by ~30% from 0 through 1500 K, there is no clear trend between its value and the temperature. The evolution of the 10-keV displacement cascades for each temperature in Ni–25%Fe is illustrated in Fig. 1. One can see that the thermal-spike lifetime obviously increases as the temperature increases at constant PKA energy. The final number of Frenkel pairs is smaller than the value predicated by the NRT model as expected. For each Ni–Fe alloy composition, we find similar temporal behaviour of the properties discussed above; thus, only a single example is shown in Fig. 1 to illustrate the typical response.

In fact, Fig. 1 offers some clue for the impact of temperature on the final number of Frenkel pairs. Therefore, to obtain a cleared picture, it is useful to compare the value of N_f at each temperature for each alloy composition, as shown in Fig. 2. As one can see from this figure, N_f exhibits a small but clear temperature dependence, with N_f decreasing as temperature increases. This temperature dependence can be attributed to the fact that high temperature allows more defect motion to take place before cooling, lengthens the thermal-spike time, and hence leads to more interstitial–vacancy recombination. This is consistent with results from previous work [17], in which irradiation damage in α-iron has been studied by MD simulation at several irradiation temperatures.

A closer inspection of Fig. 2 reveals that the Fe presence seems to increase the N_f value at low temperature; nevertheless, its influence decreases and even disappears at high temperature for these three alloy compositions. The low-temperature effect can be attributed to the threshold difference between an Fe and Ni recoil in a Ni cell. The medium thresholds for the Ni cell with Fe recoil is 6 eV lower than with Ni recoil[10]. However, the pure Ni and Ni–25% Fe alloy have almost the same N_f value, so the threshold energy difference cannot alone explain its consistency. It is more likely that it results from the relatively unstable Ni–Fe dumbbell [26] and the lower Fe threshold energy in the Ni cell. For the Ni–50% Fe alloy, the N_f value is larger than those of the other two alloy compositions in the medium temperature range. This can be attributed to the Ni–Fe and Fe–Fe dumbbells being more stable in the Fe cell than in the Ni cell [27], which limits recombination during cascade cooling. The very high temperature will counteract some effects of the different dumbbell formation energies and this may explain why the alloy composition effect of N_f is not obvious at high temperature.

3.2. Point defect clustering

Understanding the production mechanisms of large clusters of defects is of practical interest for reducing irradiation damage;

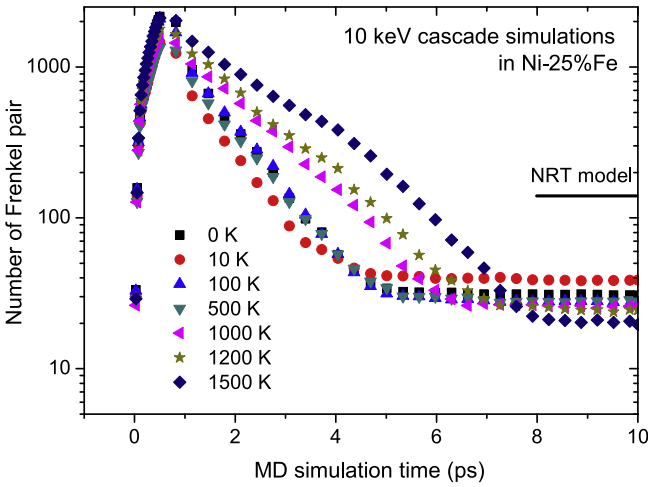

Fig. 1. Time evolution of defects formed during displacement cascades.

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