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Object Kinetic Monte Carlo calculations of electron and He irradiation of nickel

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ABSTRACT

We present results of an Object Kinetic Monte Carlo model (OKMC) of nucleation of He–vacancy complexes under irradiation of nickel. This OKMC model has been constructed using the existing atomistic information on migration energies and binding energies of vacancies, self-interstitials and He–vacancy interactions, as well as He migration from embedded atom interatomic potentials. We use this model to first study the different annealing stages of electron irradiated Ni and the influence of impurities in the recovery of damage during isochronal annealing. Then, He desorption from implanted Ni is studied for different doses and compared to existing experimental measurements.

1. Introduction

Irradiation of structural materials can alter significantly their mechanical properties. In the presence of gases, such as those appearing through transmutation in fusion irradiation conditions, an enhanced production of bubbles and voids may occur [1]. The effects on these impurities, such as He, on damage evolution is a very complex problem that depends on a large number of parameters: temperature, dose rate, He per dpa ratio, crystal structure, alloy composition and many others. One of the difficulties in modeling such processes is the need to connect different length scales, starting from the microscopic production of defects, interaction of He with vacancies and self-interstitials produced in the radiation as well as their interaction with grain boundaries and dislocations, the diffusion mechanisms for He and the kinetics of bubble and void nucleation. Many of these fundamental questions are still not fully understood.

We focus our work on He effects in f.c.c. materials, known to be more prone to swelling, and in particular in Ni, used as a surrogate material for austenitic steels. Firstly, we study defect production in Ni under electron irradiation and compare to existing experimental data as a validation for the model. Then, we study the desorption of He from Ni to understand the nucleation and stability of He–V complexes.

2. Damage accumulation in electron irradiated nickel

In order to study microstructure evolution under irradiation Object Kinetic Monte Carlo simulations were performed, based on the residence time algorithm. This method has been used extensively to study defect diffusion in many different materials and conditions [1–4]. It follows the evolution of a set of objects that can perform different types of events such as defect migration and cluster dissociation, if the probability of occurrence of each one of those events is known. Details of the simulation method are given in Ref. [4]. For the case of Ni the defects that are included in the model are vacancies and self-interstitials, including clusters of these defects, He at an interstitial position and He_nV_m clusters, where n is the number of He in the cluster and m the number of vacancies. Sinks for vacancies and self-interstitials are included as point objects with a capture radius of 1.4 nm.

The isochronal annealing of electron irradiated Ni has been studied in order to obtain the different annealing stages and compare with experimental observations. Starting with a concentration of 2 appm of Frenkel-pairs at a temperature of 4.5 K, the isochronal annealing has been followed up to 612 K. Frenkel-pairs were generated randomly in the simulation box with a distance between vacancies and interstitials of 1.3 nm. Holding times were 300 s. All self-interstitial clusters were considered mobile, with those of sizes up to three moving in 3D and larger sizes moving in 1D. Values for the mobilities and binding energies are reported in Ref. [5]. The size of the simulation box was 352 nm × 352 nm × 352 nm, with periodic boundary conditions. A concentration of sinks was introduced in the simulation box of $2 \times 10^{14}\,cm^{-3}$. Fig. 1 shows the percentage of defects as a function of temperature obtained from these calculations (solid line). From the derivative of this curve the location of the different annealing stages can be obtained. The first peak is located at ~45 K and it is related to the migration of single-self-interstitials, followed by a second peak at ~61 K related to the migration of self-interstitial clusters. At around 340 K a third peak appears that corresponds to the

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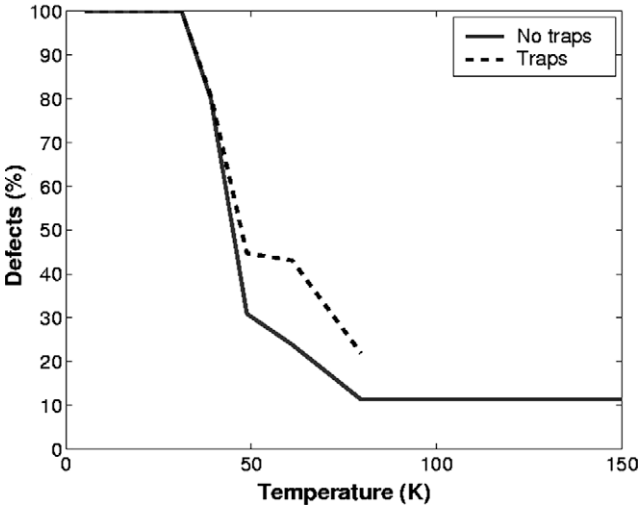

Fig. 1. Defect evolution as a function of temperature during isochronal annealing of Ni.

migration of vacancies. This is in agreement with experimental measurements where Stage I occurs at ~56 K and stage III at ~340 K [6]. Also in Fig. 1 we present results when trapping sites for self-interstitial clusters are included (dashed line). As observed experimentally [6] the presence of trapping sites changes the total recombination and the annealing stages, particularly stage II. With these calculations, therefore, we have validated the values of migration and binding energies of defects used in the model.

3. He desorption from implanted Ni

The validated model described above for vacancies and self-interstitials in Ni has been extended to include He and the formation of He–V clusters. The values for migration energies and binding energies of these complexes are those calculated by Adams and Wolfer [7] using molecular dynamics.

Using this kinetic model we have studied the desorption of He from implanted Ni in the conditions used by Edwards and Kornelsen on their experiments [8]. These experiments consisted of implanting 400 eV He ions into nickel single crystal. After implantation the temperature of the sample was increased from 300 K up to 1200 K with a ramp rate of 18.4 K/s. The number of He atoms being desorbed from the surface was measured and the time derivative of the helium partial pressure was recorded.

In order to reproduce these experiments SRIM [9] was used to compute the distribution of defects produced by the 400 eV He implantation in Ni. This was used as the input data for the OKMC calculations. Initially a room temperature annealing was performed to obtain the stable population of defects after implantation. During this room temperature annealing all self-interstitials recombine with the surface or with other defects due to their fast mobility. The implanted He interstitial atoms recombine with vacancies to form He substitutional or small He–V complexes. Once a steady state is reached the temperature is increased using the same ramp rate as in the experiments. The total number of He atoms reaching the surface during the anneal is recorded. Fig. 2 shows the total number of recombined He at the surface as a function of temperature for two different implantation doses, 5.6×10^{12} ions/cm^2 (solid line) which corresponds to the dose in the experiments by Edwards and Kornelsen [8], and at higher dose 5.6×10^{14} ions/cm^2. It can be noted that at low doses there is an initial release of He at ~650 K and a second release at ~950 K, while for higher doses He is not released until the temperature

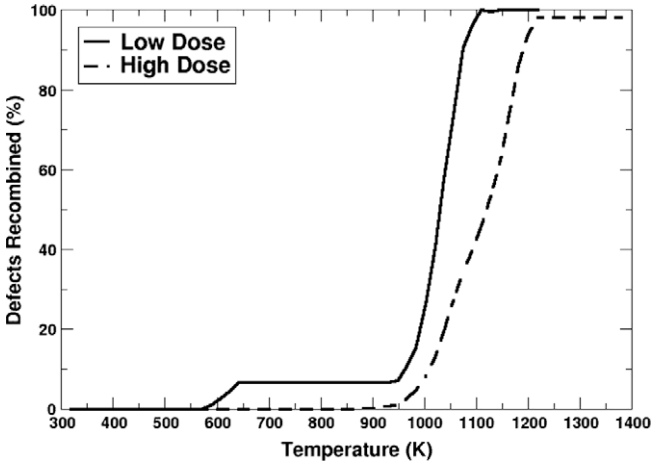

Fig. 2. He atoms recombined with the surface during annealing for two different implantation doses.

reached is ~1000 K, since the He–V complexes present are more stable.

The derivative of these curves can be compared to the experimental observations. Through different thermal helium desorption spectroscopy (THDS) experiments, three distinct peaks, named B1, B2 and B3, have been identified [6,8]. These peaks are located at temperatures of ~677 K, 835 K and 1100 K, respectively. Table 1 shows the reactions that have been associated to each of these peaks and the corresponding binding energies obtained from experiments.

Fig. 3 shows the derivative of curves presented in Fig. 2, for both cases, low and high dose of implanted He atoms in Ni. For the case of low dose two peaks are observed, as in the experimental measurements of [6,8]. The first peak corresponds to the dissociation

Table 1
Binding energies of He_nV_m vacancy clusters associated to peaks in THDS experiments. The experiments can be found in the review by Ullmaier [10].

THDS peak	Reaction	Energy experiments (eV)
B1	$He_2V \rightarrow He + HeV$	1.7–1.8
B2	$HeV \rightarrow He + V$	2.1–2.4
B3	$He_2V_2 \rightarrow HeV_2 + He$	2.8

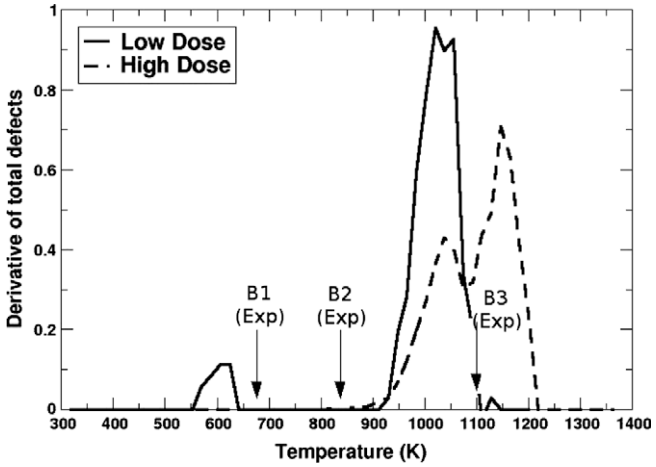

Fig. 3. Derivative of the curves in Fig. 2, showing the desorption spectra of He from Ni for two different implantation doses.

of He_2V clusters: $He_2V \rightarrow HeV + He$ which has a dissociation energy of 1.59 eV (from 1.47 eV for the binding of the He to a HeV cluster plus the migration energy of the He, 0.12 eV). This would correspond to the B1 peak in the experiment. The value found experimentally is slightly higher, between 1.7 and 1.8 eV, which explains the shift of the simulated peak to lower temperatures with respect to the experimental one, as shown in Fig. 3. The second peak observed is due to the dissociation mechanism, that is, a He at a substitutional position moves into an interstitial position: $HeV \rightarrow He + V$. The energy from the calculations is 2.68 eV (2.56 eV for the binding of HeV and 0.12 eV for the migration of He). This corresponds to peak B2, that experimentally has a significantly lower value, between 2.1 and 2.4 eV (0.3–0.6 eV difference). The reason for this discrepancy is being investigated.

For the higher dose case, only two peaks are also observed. In this case the peak due to the He_2 V cluster disappears while there is a new peak at ~1150 K. This last peak is in agreement with peak B3. This peak has been associated to the dissociation of a He atom from a He_2V_2 cluster. From our calculations, this last peak seems to be the result of the contribution of not just one single cluster but several He–V clusters, in particular, He_2V_2, He_4V_4 and He_5V_5.

4. Conclusions

Using OKMC with input data from empirical potentials we have studied the isochronal annealing of Ni irradiated with electrons and the desorption of He. Results from these calculations are in agreement with experimental measurements. Some discrepancies are found regarding the exact position of the desorption peaks particularly for the B2 peak. The input data from the model should be reviewed considering *ab initio* data, as well as further information from experimental measurements.

Acknowledgments

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