He production and induced swelling in KOYO-F

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Abstract. From preliminary results of neutron fluxes and energy spectra obtained for the vacuum vessel of the Fast Ignition Fusion Reactor KOYO-F, the distribution of Primary Knock-on Atoms (PKA), necessary to quantify defect production, has been calculated. In the presence of He these defects could induce swelling through nucleation of voids and bubbles. Kinetic Monte Carlo models are being developed to predict the evolution of these defects in different metals. As a first study we have focused on He in Ni, since there are systematic experimental results available.

1. Introduction

The production of high levels of He during operation of future fusion reactors could affect the mechanical properties of structural materials. In particular He could induce swelling of these materials due to the interaction with vacant sites in the lattice, and the stabilization of voids and formation of bubbles. Moreover, small He-stabilized defects could also act as obstacles for dislocation motion.

Therefore, it is important to evaluate the initial damage in the Fast Ignition Fusion Reactor KOYO-F, and to quantify defect production in order to study induced swelling in the reactor materials.

Consequently, the development of a physically based model to study the interactions between He and defects, and its validation with well controlled experimental measurements is needed..

2. Initial damage production in KOYO-F

A CAD-MCNP methodology for 3D neutronic calculations has been applied to the Fast Ignition Fusion Reactor KOYO-F in order to calculate the neutron fluxes and energy spectra in each section of the chamber, including the vacuum vessel. These results could be used to study how radiation affects the mechanical properties of the materials used in the vessel.

Following the previous referenced calculations, figure 1 shows the neutron energy spectra just at the beginning of vacuum vessel. These preliminary results show that the total flux is $5.45 \cdot 10^{12}$ n·cm^{-2} · s^{-1} and the maximum values of flux are found from lowest neutron energies (~eV) to energies in the range of 20 keV.

From this neutron energy spectra the Primary Knock-on Atoms (PKA) emerging from the nuclear reactions in the vacuum vessel material, which is a ferritic steel (FeCr based alloy), have been determined. These calculations have been performed using the SPECTER[2] code and the results are the first step to quantify defect production. Figure 2 shows integral primary recoil spectra versus

energy for iron and nickel under neutron energy spectra from figure 1. The irradiation period was a year. Concerning these preliminary results it can be considered that all primary recoil energies are lower than 100 keV. The values for He rate production obtained by SPECTER are 4.75 appm/dpa in iron and 27.25 appm/dpa in nickel. These results show that nickel is a more prone material to swelling than iron.

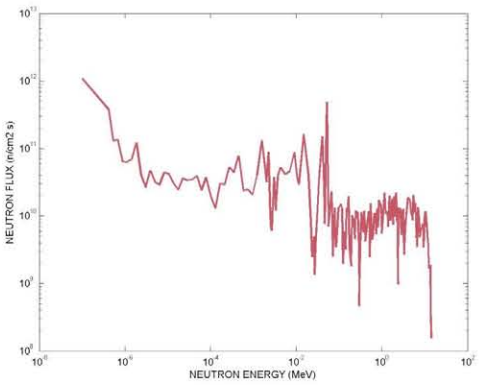

Figure 1. Neutron energy spectra in KOYO-F vacuum vessel

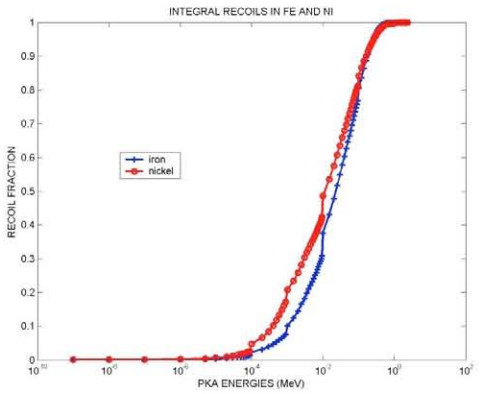

Figure 2. Integral primary recoil spectra versus energy for iron and nickel under neutron energy spectra from KOYO-F.

3. Kinetic models for He effects in irradiated materials

Our goal is to develop a physically based model for He diffusion and interaction with irradiation produced defects. This model could be applied to study void and bubble nucleation in b.c.c. and f.c.c. metals.

Rate theory models have been used to study He diffusion and He-V cluster formation in Fe and were able to reproduce experimental measurements of He desorption.

However, the number of well-controlled experiments in Fe and Fe-alloys is limited. For this reason, and as a first test study of our kinetic Monte Carlo model for He diffusion, we have selected He in Ni where experimental data is available, particularly those performed by Edwards

These experiments consisted of implanting 400eV He ions into nickel crystal. After implantation the temperature of the sample was increased from 300K up to 1200K 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.

Two peaks are observed in this experiment, named B1 and B2 . The B1 peak is believed to be associated to the dissociation of a He2V cluster, that is a cluster with 2 He atoms in a vacant site. This dissociation occurs by the cluster emitting a He atom. The B2 peak is believed to be due to the dissociative mechanism by which a He at a substitutional place moves into an interstitial place leaving a vacancy behind: HeV He + V. Through different thermal helium desorption spectroscopy (THDS) experiments, like this one for low energy He implantation in Ni, three distinct peaks, named B1, B2 and B3, have been identified These peaks are located at temperatures of ~ 677K, 835K and 1100K respectively.

In order to reproduce these experiments we have used a kinetic Monte Carlo model with input data from molecular dynamics or *ab-initio* calculations.

Firstly, SRIM is used to compute the distribution of vacancies for 400eV He in Ni. This distribution together with the distribution of He are shown in Figure 3. The self-interstitial distribution assumed is just the vacancy distribution shifted. Due to the one-dimensional migration of self-interstitials and self-interstitial clusters in Ni and the low implantation energy, most of these atoms recombine with the surface at room temperature and only a small percentage recombines with

vacancies. Therefore, the exact initial distribution of self-interstitial atoms is not relevant under these conditions.

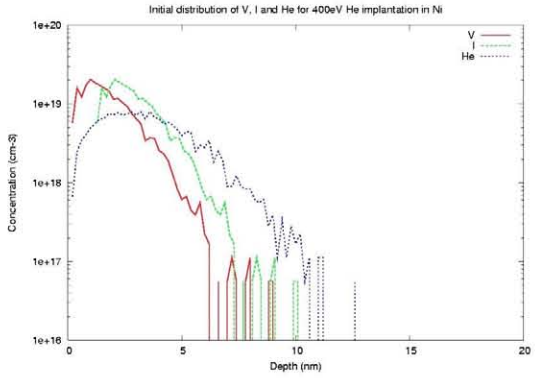

Figure 3. Distribution of V and He obtained from SRIM for a 400 eV He implant in Ni.

In order to study the long term evolution of these defects and their migration during the temperature ramp we have used kinetic Monte Carlo calculations. The input data required for these calculations are the migration energies and binding energies of different defects. The values used in this work are those calculated by Adams and Wolfer using molecular dynamics, Almazouzi et al also with molecular dynamics and by C. Domain using ab initio calculations.

Figure 4 shows the total number of He atoms reaching the surface during the temperature ramp obtained from the kMC calculations. The same conditions as in experiments by Edwards were used in these calculations. It can be noted that there is an initial release of He at ~ 650K and a second release at ~ 950K.

Calculating the first derivative of this curve with temperature (figure 5) we can obtain information that can be compared to the experimental measurements. Two peaks are observed, in agreement with the experimental observations. The calculations show that the first peak, B1, corresponds to the dissociation 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). The value found experimentally is slightly higher, between 1.7 and 1.8eV, which explains the shift of the simulated peak to lower temperatures with respect to the experimental one, as shown in figure 5. The second peak observed is due to $HeV \rightarrow He + V$. 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). The value obtained experimentally is significantly lower, between 2.1 and 2.4 eV (0.3 – 0.6 eV difference). The existence of only two peaks in the full calculation of implantation and desorption of He, in agreement with experimental observations, is quite relevant. It demonstrates the existence of predominant reactions in this system, which is not necessary the case in other materials, such as Fe, where experimentally many different desorption peaks are observed [9]. The discrepancies between experiments and simulations could be due to different reasons. On one hand slight differences in the binding energies of defects used in the calculations could result in significant shifts in temperature On the other hand differences in the actual implantation dose and the one used in the simulations could also change the position of the desorption peaks.

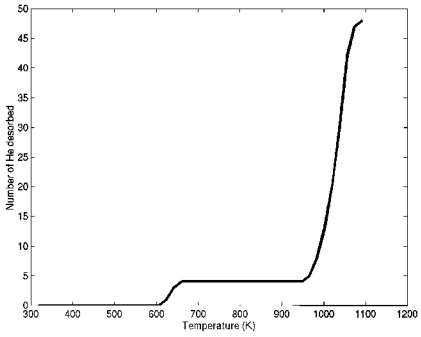

Figure 4. Total number of He atoms reaching the surface during the temperature ramp.

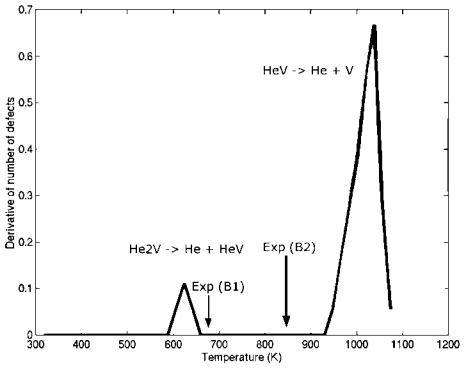

Figure 5. First derivative of the curve of figure 4.

4. Conclusions

As a first step to quantify defect production and characterize the initial damage production in KOYO-F vacuum vessel the distribution of PKA's in iron and nickel has been obtained, taking into account previous calculations of neutron fluxes and energy spectra. The preliminary results obtained show that all primary recoil energies are lower than 100 keV. The values for He rate production are also shown for both materials.

A physically based model for He diffusion and interaction with irradiation produced defects is being developed using kinetic Monte Carlo with input from molecular dynamics or *ab-initio* calculations.

The model applied to the study of He desorption from Ni at low implant energies and low dose shows two peaks in agreement with experimental observations. These peaks correspond to HeV→He +V and He_2V→He +HeV. This model is being extended to higher doses and other materials.

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