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# Defect Production in α-Iron Irradiated by Fission and Fusion Neutrons

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## Abstract

We present the results of a molecular dynamics (MD) simulation of the damage production in iron under two irradiation conditions such as those in the commercial pressurized water reactors (PWR) and fusion power reactors. Two sets of neutron spectra include a commercial PWR neutron spectrum at the 0-T reactor pressure vessel position and a DT fusion reactor (ITER) first wall spectrum. The spectral average energy of the primary knock-on atoms has been obtained from the SPECTER code, which is 5.3 keV for PWR and 7.4 keV for ITER. These were used as input for the MD simulation in which cascades of 5.3 keV at 290$^{o}$C and 7.4 keV at 500$^{o}$C have been simulated and quantitatively compared. No significant difference was found in the primary damage state between the two conditions. The high dose rate, expected in the fusion reactor environments, may be the main source of radiation damage.

## 1. Introduction

The fusion reactor environment is unique and few data exist on the behavior of materials under irradiation. The primary threat of materials exposed to a fusion environment is a high flux of fast neutrons escaping from the fusion reaction. A commercial fission reactor spectrum has a small amount of neutrons above 1 MeV outside the core region, while a deuterium-tritium (DT) fusion neutron spectrum has a peak at about 14 MeV. It is expected that the high-energy neutrons will in turn produce high-energy primary knock-on atoms (PKAs), followed by displacement cascades. In addition, a high neutron flux could lead to an increase in the production of the transmutation elements. These differences in the radiation environment do not permit the use of fission reactor data in estimating the fusion reactor data.

Various structural materials have been considered over the past 30 years for fusion reactor applications. In the selection of structural materials, a number of factors are taken into account: unirradiated mechanical properties, radiation damage, chemical compatibility, material availability and fabricability, and the nuclear property, etc [1]. Low-activation ferritic steel is one of several candidate materials for the first wall of a fusion device. Therefore, it is imperative to understand how radiation damage is produced and accumulated in iron-based alloys under fusion environments. Transmission electron microscopy (TEM) studies have made a contribution to characterizing the microstructural features produced by irradiation. However, the following two facts limit the application of electronic microscopy and irradiation experiments for a radiation damage study, which are, that the irradiation-produced defects are below the TEM resolution limits and the fusion neutron sources are not currently available [2]. The present paper is intended to simulate the primary damage production irradiated by fusion neutrons and to compare the calculation results with those by the fission neutrons. Molecular dynamics (MD) method was applied for simulating the formation and evolution of the displacement cascades. The two input parameters, characterizing the fusion and fission neutron conditions, are the temperature and the average PKA energy. From the MD simulations, the distribution of the clustering formation has been extracted and compared to investigate the difference in the primary damage state. In addition, in order to treat the high-flux effect on the primary damage, that is fusion neutron irradiation, we simulated the displacement cascade with the point defects present. It is probable that the presence of the point defects in crystalline materials enhance the formation and development of the unfavorable microstructures, which result in the degradation of the materials. In this paper, we present the difference in primary damage production by fission and fusion neutrons and the potential effect of the neutron flux on the damage production using MD simulations.

## 2. Methods

Prior to MD simulations, the basic radiation damage parameters were extracted from the SPECTER code calculation [3], of which the spectral-averaged PKA energy is our primary interest for the given irradiation conditions. Two sets of neutron spectra represent the irradiation conditions such as the commercial pressurized water reactor (PWR) and the fusion power reactor. The neutron spectra used here are shown in Figure 1, which serve as the input to the SPECTER code calculation. The facilities illustrated are: the ITER first wall [4], and the zero-thickness throughout the reactor pressure vessel of a PWR, currently operating at the Younggwang nuclear power plant in Korea. The difference in neutron spectra is caused by the neutron source term. The neutrons produced by the DT reactions have a peak energy of 14 MeV, while the neutrons produced in the $^{235}$U fission reaction emerge with a distribution of energies, with the average energy being about 2 MeV. In addition, a big difference could be seen in the neutron flux. The fast neutron ($E_n$ > 1 MeV) flux in the ITER is about 450 times greater than that in the PWR, which is influential in inducing the displacement cascade reactions. The spectral-averaged PKA energies for iron, obtained from the SPECTER calculation, are 7.4 keV for ITER and 5.3 keV for PWR. Aside from accurately analyzing the PKA energy spectrum, we have simulated the displacement reactions using one value of the PKA energy for each irradiation condition. This procedure is sufficient to obtain the average behavior at the given conditions by repeating the same simulations.

It is not simple to determine the operating conditions for the ITER because it depends on the specific reactor design. Accordingly, the simulating temperature was determined on the basis of the maximum operating temperature limits for a given structural materials. The maximum operating temperature limit for the structural materials in the fusion reactor is controlled by such mechanisms as thermal creep, helium embrittlement, void swelling, and corrosion resistance [5]. In this case, the upper temperature limit for ferritic-martensitic steels is about 500$^{o}$C, which has been set to be the MD simulation temperature for the fusion neurons. The MD simulation temperature for the fission neutron was fixed at 290$^{o}$C, corresponding to the normal PWR operating temperature.

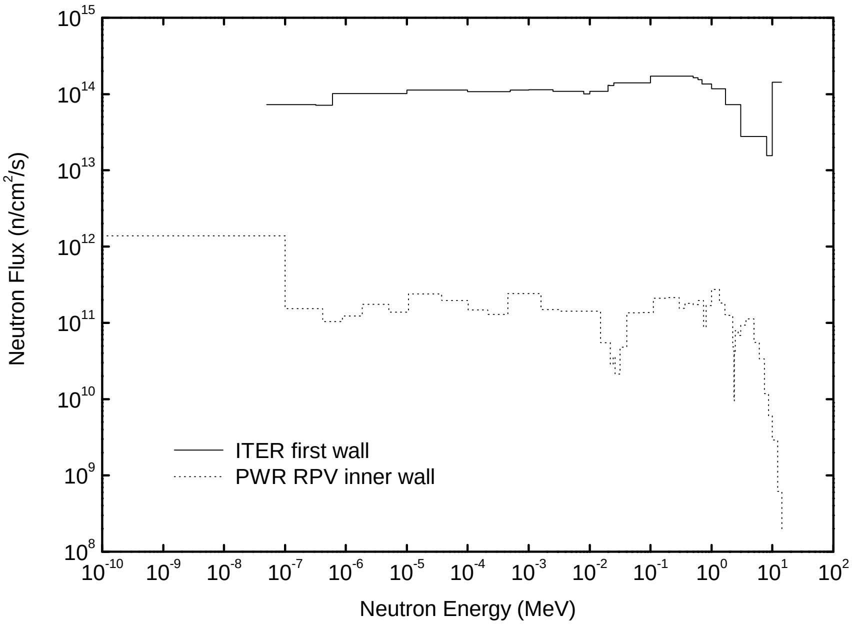


Figure 1. Neutron spectra in the two irradiation environments: ITER first wall (DT fusion) and PWR reactor pressure vessel inner wall (thermal fission).

Simulations of displacement cascades were carried out with the MD code, MOLDY [6]. The MOLDY has been used widely for simulations of displacement cascades in metals. The classical equations of motion for atoms are integrated via a Gear 4-value predictor-corrector algorithm [7] and the many-body interatomic potential for $\alpha$-iron, derived by Finnis and Sinclair [8], is embedded in the MOLDY. Since the MOLDY does not account for the energy loss due to electronic excitation and ionization, the initial energy given to the PKA needs to be calculated. This kinetic energy, used as an input energy in the MD calculation, is analogous to the damage energy ($T_{dam}$) in the standard NRT model [9]. The relationship between the PKA energy, $E_p$ and $T_{dam}$ is expressed as,

$$\frac{T_{dam}}{E_p} = \frac{1}{1 + \lambda\ w(E^*)} \tag{1}$$

where, $\lambda$ is given by $\lambda = 0.0876\,Z^{1/6}$, Z = atomic number. The function $w(E^*)$ and its variable $E^*$ can be written in terms of $E_p$ and Z:

$$w(E^*) = E^* + 0.402\,(E^*)^{3/4} + 3.4\,(E^*)^{1/6} \tag{2}$$

$$E^* = \frac{E_p}{0.0869\,Z^{7/3}}, \quad E_p \text{ in keV} \tag{3}$$

The PKA energy of 7.4 and 5.3 keV corresponds to the 5.65 and 4.09 keV damage energy for iron, respectively.

The cascade simulations have been performed until the recombination of interstitial and vacancy is finished. However, the atomic block does not return to a complete thermal equilibrium after the recombination phase due to a high temperature. Accordingly, we run the code until the number of point defects becomes stable. In the present case, about 10 ps of simulation time is required to complete the computation with 128,000 atoms. For a given PKA energy, six simulations have been carried out with different initial conditions, which are the three directions of incident PKA - [135], [111] and [100], and two different lattice positions. The same conditions are applied to both the fusion and fission irradiation environments. The parameter of our interest is the number of point defects that survive from the cascade recombination. Such defects that are free to migrate over relatively long distances play an important role in the formation of a radiation-induced microstructure. The density distribution of the point defect clusters is also important in that these small clusters act as an embryo for the development of large defects.

## 3. Results

The size distribution of the residual point defects is calculated from the MOLDY output by averaging the six simulation results. The size distribution of the point defect clusters – interstitial and vacancy are plotted in Figure 2. The similar trend in clustering statistics could be observed for both the fusion and fission environments. In spite of a high PKA energy for ITER irradiation, there is no significant difference in the number of residual point defects. High temperature contributes to the recombination of the point defects by enhancing the thermal motion. For interstitial clustering, about 30 % of the residual interstitials become single isolated defects, while most residual defects tend to form clusters albeit small in size. In ITER irradiation, the formation of the di-interstitials is predominant. The clustering formation of the interstitials is important in that these defects are thermally stable and can migrate away in groups from the parent cascade region to be absorbed at sinks. In contrast, about 70 % of the residual vacancies remain as single defects in the ITER and PWR irradiation. As seen from Figure 2, the distributions indicate that the primary damage production in an ITER environment should be similar to that generated in a PWR.

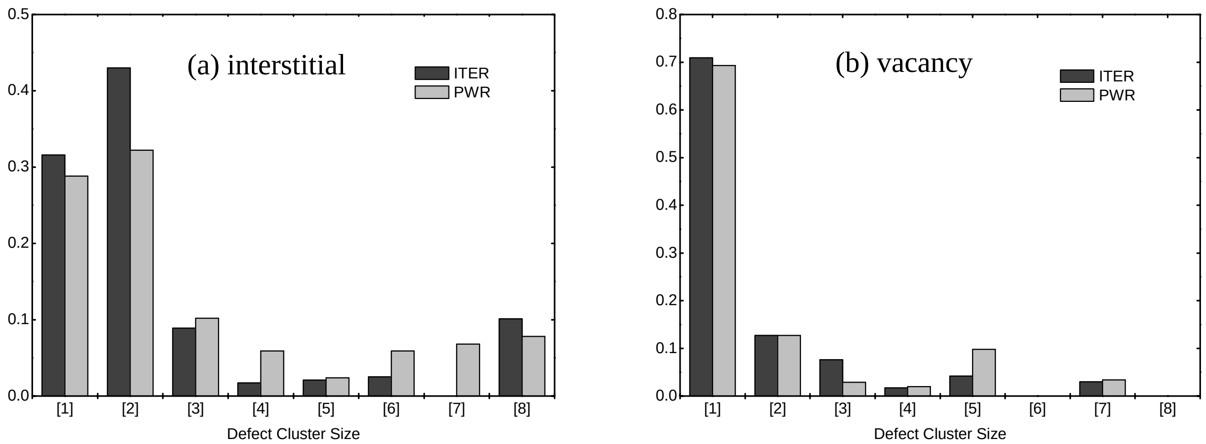


Figure 2. Size distribution of residual point defects for (a) interstitial and (b) vacancy ; results of MD simulations at 500°C, $E_p$= 7.4 keV for ITER and at 290°C, $E_p$ = 5.3 keV for PWR.

The major distinction between the ITER and PWR irradiation environments can be found from the difference in the neutron flux. Although it is not possible to accurately simulate the multiple displacement cascades using the MD code, the relative comparisons of the dose rate effect on the primary damage may be made with the MD computation. For example, more PKAs will be created per unit time through the collision between the neutrons and lattice atoms for the higher dose rate irradiation. Therefore, it is highly probable that the displacement reactions take place more frequently within the specified region. We deal with the high dose-rate irradiation by simulating the displacement cascades with the point defects included at the beginning. The same calculations have been carried out using the MOLDY in an ITER environment except for the fact that several point defects were located previously at given positions. The initial locations of the interstitials should be close to their equilibrium values. Otherwise the computation does not converge. It is critical to maintain the stability of the calculation when point defects are included at the beginning.

The examples of displacement cascade evolution in an ITER environment are illustrated in Figures 3 and 4 for a low-dose rate and a high-dose rate irradiation, respectively. The former visualizes the development of the displacement cascade from the perfect lattice structure of $\alpha$-iron. The number of point defects reaches a peak at time t = 0.51 ps and then decreases gradually by the athermal relaxation process. The similar behavior could be observed in the high dose-rate simulations, shown in Figure 4. Initially, ten point defects, five of each the interstitial and vacancy, have been placed at specified positions which are in the vicinity of the PKA location. The presence of the point defects prior to a PKA entry alters the displacement morphology to some degree. Not only does the final number of residual defects increases but they are also spatially distributed to a wide region, which can be verified by comparing the final pictures in Figures 3 and 4.

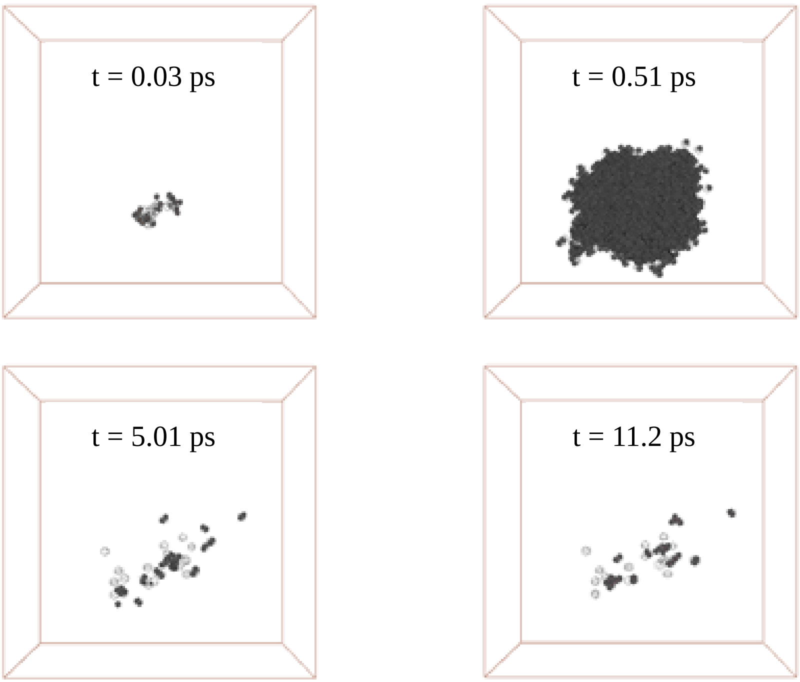


Figure 3. Development of a 7.4 keV cascade at 500$^{o}$C from the perfect lattice structure – low dose rate irradiation. The block size is $40a_o$x$40a_o$x$40a_o$, and the initial PKA direction [135]. Vacancies and interstitials are denoted by light and dark spheres, respectively.

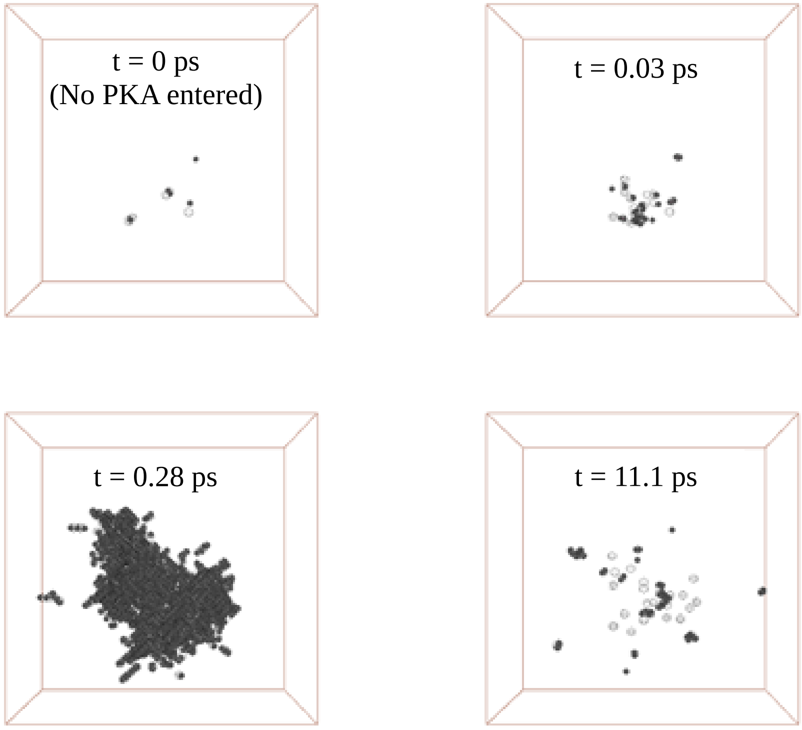


Figure 4. Development of a 7.4 keV cascade at 500$^{o}$C with initial point defects included – high dose rate irradiation. Refer to the captions in Figure 3 for illustration.

The size-distribution of the point defect clusters in an ITER environment averaged over the six cascade simulations is shown in Figure 5. There is a distinction in the primary damage state between the two cases – with and without the initial defects. The simulation with the initial defects included corresponds to the high neutron flux irradiation, which reflects irradiation conditions similar to the actual ITER environment. Overall, for the case of a high flux irradiation, the total number of residual defects at the final stage of the simulation (t > 10 ps) increases by about 10%. This is of no importance because the number of point defects fluctuates to a degree at the high temperature. It is, however, found that a greater number of residual defects tend to form isolated defects rather than clusters, which is dominant for interstitials.

## 4. Summary and discussion

The results of the MD cascade simulations for iron are presented under conditions relevant to the ITER fusion reactor first wall. Among various structural materials considered for the fusion application, we have selected iron-based alloy such as reduced activation ferritic-martensitic steel and analyzed the primary damage production. And, unlike other MD simulations, the spectral-averaged PKA energy obtained from the SPECTER code was used for the cascade simulation. The primary damage parameters derived from the MD results exhibit a similarity between the ITER and PWR irradiation. No significant difference was found in the total number of point defects created after the

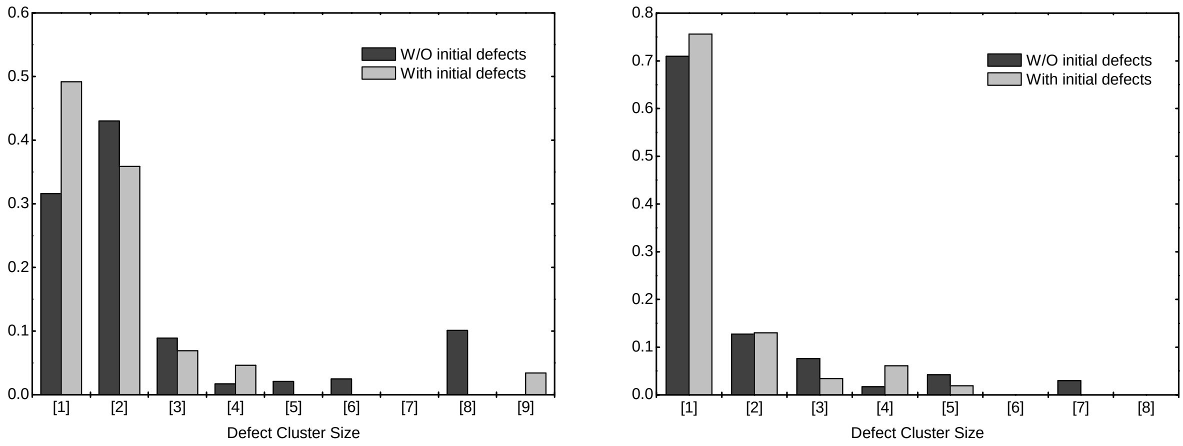


Figure 5. Size distribution of residual point defects for (a) interstitial and (b) vacancy; both results from MD simulations for ITER irradiation conditions with and without initial defects.

displacement cascades in spite of the difference in the PKA energy. A high temperature in the ITER environment might enhance the cascade annealing. It is believed that the primary damage production at the ITER first wall is not as severe as was expected. Such a qualitative explanation is not sufficient to warrant the integrity of iron irradiated by fusion neutrons because the MD simulation can only simulate the atomic behavior occurring within tens of picoseconds.

Attempts were made at investigating the effects of a high dose rate on the primary damage in the ITER environments. The presence of initial defects in the displacement reactions increases the number of primary defects and extends the area of damage. A preferential tendency to form isolated interstitials was observed in this study. Although it is not possible to directly conclude from this simulation the role of the isolated defects, the lesser production of the defect clusters seems to decrease the probability of nuclei formation for the extended defects such as dislocation loops and microvoids. Such an explanation is only qualitative at this point, and further analysis will be required to determine the role of isolated point defects.

## 5. Acknowledgments

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## 6. References

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