Primary Damage Production of α-Iron in PWR and SFR Environments

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1. Introduction

The primary threat of materials exposed to a nuclear reactor environment is a high flux of fast neutrons produced from the fission reaction. A commercial pressurized water reactor (PWR) spectrum has a small amount of neutrons above 1 MeV outside the core region, while relatively sodium fast reactor (SFR) has a large amount of fast neutrons. It is expected that the fast neutrons will in turn produce high-energy primary knock-on atoms (PKAs), followed by displacement cascades. These differences in the radiation environment do not permit the use of thermal reactor data in estimating the fast reactor data.

The present paper is intended to simulate the primary damage production irradiated by neutrons in a SFR environment and to compare the calculation results with those in a PWR one. Molecular dynamics (MD) method was used for simulating the evolution of the displacement cascades. The two input parameters, characterizing the SFR and PWR conditions, are the temperature and the average PKA energy. From the MD simulations, the distribution of the point defect clustering formation has been extracted and compared in order to investigate the difference in the primary damage state. It is probable that the presence of the point defects in crystalline materials enhances the formation and development of the unfavorable microstructures, which ultimately affect the degradation of the materials.

2. Methods

Prior to MD simulations, the basic radiation damage parameters were extracted from the SPECTER code calculation [1], of which the spectral-averaged PKA energy is our primary interest for the given irradiation conditions. Two sets of neutron spectra were obtained; one represents the neutron spectrum on the inner surface of the pressure vessel steels in a commercial PWR and the other stands for the neutron spectrum on the outer core in a SFR. The normalized neutron spectra used here are shown in Fig. 1, which serve as the input to the SPECTER code calculation. A big difference could be seen in the neutron flux. The fraction of fast neutron (E_n > 1 MeV) flux in the SFR is about 3.3 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 38.2 keV for SFR and 5.3 keV for PWR. Aside from accurately analyzing the PKA energy spectra, 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.

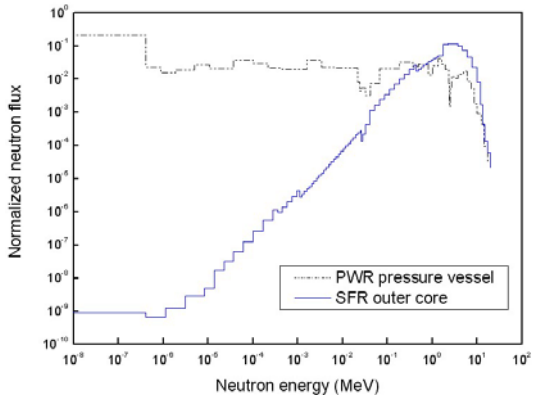


Fig.1 Normalized neutron spectra in two environments: PWR pressure vessel and SFR outer core

Simulations of displacement cascades were carried out with the MD code, called MOLDY [2]. 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 and the many-body interatomic potential for α-iron, derived by Finnis and Sinclair, 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 modified. 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 [3]. The relationship between the PKA energy, E_p and T_{dam} is expressed as,

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

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

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

$$E^* = \frac{E_p}{0.0869\, Z^{7/3}}, \; E_p \text{ in keV} \qquad (3)$$

The PKA energy of 38.2 and 5.3 keV corresponds to the 25.8 and 4.1 keV damage energy for iron, respectively.

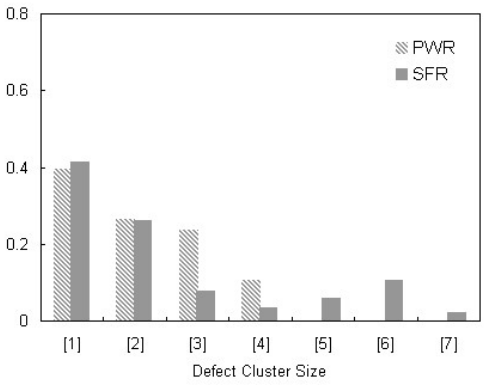
The cascade simulations should be continued until the recombination of interstitial and vacancy is finished. However, the atomic block does not return to a complete thermal equilibrium after the recombination phase due to high temperature. Since the expected operating temperature for a SFR and a PWR is 550^{o}C and ~300^{o}C respectively, the number of residual point defects fluctuates more or less. Accordingly, we terminated the simulation after 10,000 steps. For a given PKA energy, five or more simulations have been carried out with different initial condition of the initial direction of PKA. The same conditions are applied to both SFR and PWR environments. The parameter of our interest is the number of point defects that survive from the cascade recombination and the distribution of the point defect clusters. It is likely that the small clusters act as an embryo for the evolution of large defect, including precipitates, dislocations, voids, etc.

3. Results

The size distribution of the point defect clusters – interstitial and vacancy are plotted in Fig. 2. The similar trend in clustering statistics could be observed for both the SFR and PWR environments. The difference in PKA energy leads to a big difference in the average number of residual point defects: 19 for PWR and 69 for SFR. There is, however, not a significant difference in the distribution of residual point defects. As shown in Fig. 2, the fraction of point defect clustering is very similar except that big-size clusters are found for the SFR environments. For vacancy clustering, the formation of the multiple-vacancy is important in that these defects can act as an embryo for the void formation. This void swelling is one of potential problems at the high temperature under irradiation.

4. Conclusions

The results of the cascade simulations for α-iron are presented in conditions relevant to the SFR. Not a big difference between SFR and PWR environments was found in the normalized distribution of defect clustering in spite of a difference in the PKA energy. The creation



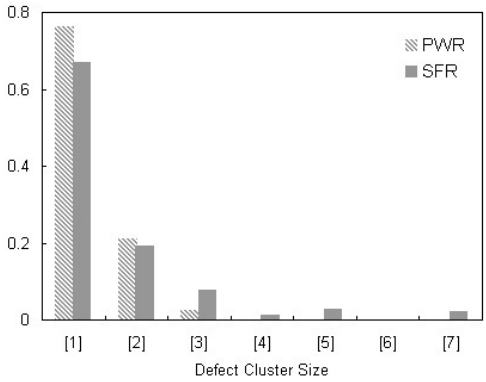


Fig. 2 Size distribution of point defect clusters for (a) interstitial and (b) vacancy; results from the MD calculations at 550^{o}C for SFR and ~300^{o}C for PWR.

of big-size defect clusters in SFR conditions seems to increase the probability of microstructure formation. Further analysis, such as kinetic Monte Carlo simulations and reaction rate theory modeling, is required to determine the role of residual defects.

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