Estimation of primary radiation damage cross sections for iron

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1. Introduction

Radiation damage in materials is caused by the energy transfer of a high-energy incident particle to the target atoms, which finally results in the redistribution of target atoms. During the nuclear reactor operation, wide range of neutron spectrum is produced, which affects the microstructure of structural materials and finally results in their property changes in a direct and/or indirect way. The two most common parameters used for characterizing the cumulative exposure of a material to irradiation are the particle fluence and absorbed dose. The particle fluence, usually in units of cm^{-2}, depends on the irradiation source and can be determined by averaging over a certain area or volume. The absorbed dose, in units of energy, is dependent on several variables, including particle-type, fluence, energy spectrum and the target material. Actually, the absorbed dose includes more information about the irradiation environment than the particle fluence. Both parameters are used as independent variables to represent radiation exposure in experiment and for reactor structure. Both parameters may be used as a damage correlation parameter in attempts to correlate data from different irradiation environments. The particle fluence, however, is limited when the type of particle is not the same.

The primary damage in structural materials arises from an atomic displacement cascade which involves a number of collisions between the lattice atoms following the introduction of an energetic particle. Such cascade leads to the production of many point defects, which are vacancy- and/or interstitial-type defects. In defining the amount of displacement damage to material, the secondary displacement model of Norgett, Robinson, and Torrens (NRT) has been a standard in the nuclear materials research society since 1975 [1]. The major physical parameter in the NRT model is the damage energy, which is the energy dissipated in the successive collisions among lattice atoms. The damage energy provides a convenient method of estimating the number of atomic displacements per atom (dpa). Although the NRT model does not express the actual number of vacancies and interstitials formed, the model is well within an order of magnitude of the actual quantity which was verified by modern molecular dynamics (MD) simulations and cryogenic irradiation tests. In this paper, we calculated the primary radiation damage cross sections which implicate the net damage production due to neutron irradiation to structural material. We refer to the MD simulation results given in the published literature and apply the latest ENDF/B-VII cross section library. This work was performed for iron which is a main element of structural materials in a nuclear reactor. The developed methods in

this work will enable us to accurately predict the net damage production as a result of neutron irradiation.

2. Primary Radiation Damage Parameters

In this section some of primary radiation damage parameters, used commonly to quantify the amount, are described. The parameters include dpa, displacement cross section and damage energy production cross section.

2.1 Displacement per atom (dpa)

Displacement per atom (dpa) represents the calculated number of recoil atoms that are displaced from their lattice sites as a result of particle collision. The *dpa* rate (dpa/s) due to neutron irradiation is given by:

$$\text{dpa rate} = \sum \phi(E) \cdot \sigma_{dis}(E) \tag{1}$$

where $\phi(E)$ = neutron spectra, $\sigma_{dis}(E)$ = displacement cross section (barn) and E = incident neutron energy.

The displacement cross section is defined as a probability of displacing atoms from their lattice sites by an incident particle, which depends on the incident neutron energy and microscopic cross sections, primary recoil atom energy distributions and secondary recoil atom probabilities. Mathematically this is expressed as:

$$\sigma_{dis}(E) = \sum_i \sigma_i(E) \int_{T_{min}}^{T_{max}} f_i(E,T) \cdot \nu_{NRT}(T)\ dT \tag{2}$$

where T = recoil atom energy, $\sigma_i(E)$ = microscopic cross section for i-type reaction, $f_i(E,T)$ = neutron-atom energy transfer kernel and $\nu_{NRT}(T)$ = secondary displacement function. The energy transfer kernel stands for the probability that a particle of energy E will impart a recoil energy T to a struck lattice atom and the secondary displacement function is the number of displaced atoms resulting from such a collision [2]. By multiplying the displacement cross section and given neutron spectra, we can readily calculate the *dpa* values, that is, the amount of neutron damage to materials.

2.2 Damage energy production cross section

The number of dpa depends on the total available energy and the energy required to displace an atom from its lattice position, called the displacement threshold energy, E_d. The energy available to cause atomic displacements can be obtained from the NJOY nuclear data processing system [3]. NJOY has a module HEATR which can calculate the damage energy using NRT model by tracking the recoil energy from all possible neutron reactions [1]. One of outputs from HEATR is the damage energy production cross section in units of eV-barn, which is given by:

$$D(E) = \sigma(E)\int g(E \rightarrow E') \cdot P(E')\,dE' \qquad (3)$$

where $g(E \rightarrow E')$ = angle-integrated energy distribution from the incident neutron energy E and P(E') = damage partition function. Dividing Eq. (3) by E_d gives the displacement cross section of Eq. (2).

2.3 Molecular dynamics (MD) simulations – Displacement cascade

The MD method is a powerful technique for simulating displacement cascades in ordered materials. Since these phenomena cannot be directly observed in experiments, the available information about primary damage comes from the computational simulations. Two parameters are of primary interest to the MD cascade simulations: the number of point defects that survive after in-cascade recombination is finished, and the fraction of the surviving point defects that are formed in clusters. The former is important because the residual defects can make a contribution to the subsequent microstructural formation. The temporal evolutions of the displacement reactions are shown in Fig. 1, which was obtained from the MD simulations. We can find that only a small fraction of point defects survived within tens of pico-seconds.

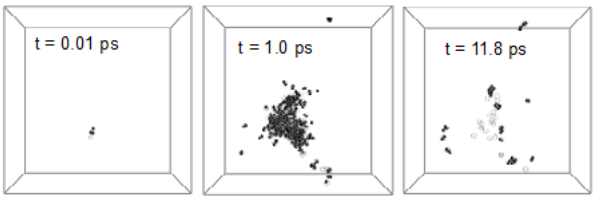

Fig. 1. Temporal evolution of displacement cascades in iron at 290°C. (dark dot - interstitials, white dot - vacancies)

The surviving MD defects can be another parameter to define the primary radiation damage. While the surviving defect fraction is a function of damage energy, its temperature dependency is weak. Under the assumption that the damage energy is equivalent to the MD cascade energy E_{MD}, the surviving defect fraction (η) can be plotted in Fig. 2 [4]. The trend curve was derived from a number of MD simulations for various MD cascade energy, which may be applied to calculate net damage production cross sections. The line drawn in the figure can be approximated by:

$$\eta(E_{MD}) = 0.5608\,E_{MD}^{-0.3029} + 3.227\times10^{-3}E_{MD} \qquad (4)$$

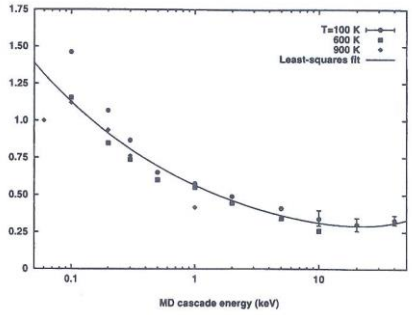

Fig. 2. Average point defect surviving fraction as a function of MD cascade energy [3]

3. Calculation of Damage Cross Sections

The HEATR module generates pointwise radiation damage energy production cross section (eV-barn) which represents the recoil energy available to cause the displacement cascade. From this cross section, we can readily derive the displacement cross section. The damage energy production cross section from the NJOY calculation and the displacement cross section for Fe are shown in Fig. 3. It is found that thermal neurons are capable of causing displacement damage as well as fast neutrons.

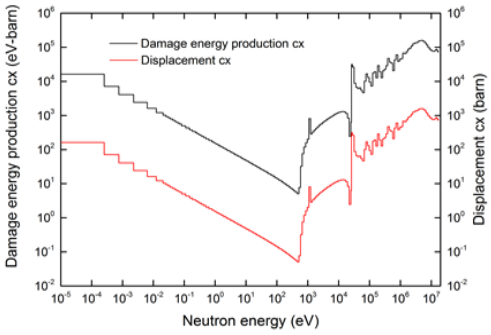

Fig. 3. Damage energy production cross sections (black) and displacement cross section (red) for iron. (E_d for Fe = 40 eV)

It is plausible to derive the net damage production cross section from the displacement cross section, which can be expressed in a mathematical way such as:

$$\sigma_{dis}^{net}(E) = \sum_i \sigma_i(E) \int_{T_{min}}^{T_{max}} f_i(E,T) \cdot \nu_{NRT}(T) \cdot \eta(T)\ dT \qquad (5)$$

The surviving defect fraction, Eq. (4), in combined with the displacement cross section, Eq. (2), which gives the parameter in determining the amount of net damage production. Such net damage production cross section, Eq. (5), will be another damage parameter.

4. Discussion

In estimating the amount of radiation damage, efforts have been made to find an alternative to the NRT model that accurately takes into account primary damage more and possibly improves damage correlation. In this respect, we investigated the primary radiation damage parameters on the basis of the NRT model, currently in use. Two damage parameters were taken into account from the NJOY system, which were displacement cross section and damage energy production cross section for iron. We suggest another primary radiation damage parameter, which is called net damage production cross section. This parameter will be derived by including the results of the MD cascade simulations. It is believed that this parameter will be useful for correlating damage mechanisms.

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