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Analysis of Proton Induced Material Damage Using the DPA Cross-sections Based on NRT and BCA-MD Models

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1. Introduction

Mechanical properties of the materials used in nuclear reactor and accelerator facilities can be changed by radiation irradiation, and their damage can affect the lifetime and the safety of these facilities. The level of radiation induced material damage is mainly quantified by using the unit of Displacements Per Atom (DPA), and particularly, the displacement cross-section is used for characterizing/analyzing the radiation damage from incident neutrons and charged particles [1].

Not long ago, the standard Norgett-Robinson-Torrens (NRT) model had been applied to produce the nuclear data due to its simplicity and implementation in commonly used codes, such as NJOY and MCNP codes. However, the evaluations based on NRT model represent the severe disagreement with experimental data and more accurate calculations [2]. This problem increases the need for the evaluation of the nuclear data for structural materials on the basis of advanced models, and they are recently reproduced by the binary collision approximation model and the results of the molecular dynamics (BCA-MD) [3].

Hence, the evaluations with existing and new nuclear data are performed/compared in this study. It is assumed that a high energy proton beam is directly moved to the target, and a series of calculations are performed by using MCNPX code [4].

2. Methods and Materials

The general expression for the displacement cross-section can be written as follows [5];

$$\sigma_d(E) = \sum_i \int_{E_d}^{T_i^{\max}} \frac{d\sigma(E, Z_T, A_T, Z_i, A_i, T_i)}{dT_i} \times \eta(Z_T, A_T, Z_i, A_i, T_i) N_{NRT}(Z_T, A_T, Z_i, A_i, T_i) dT_i \quad (1)$$

where E is the incident radiation energy, $d\sigma/dT_i$ is the recoil atom energy distribution, and Z and A are the atomic and the mass numbers, respectively (T: target atom, i: recoil atom). η is the defect production efficiency, and N_{NRT} is the number of defects predicted by NRT model which is as follows;

$$N_{NRT} = \frac{0.8 \times T_{dam}}{2E_d} \quad (2)$$

where T_{dam} is the damage energy equal to the energy transferred to lattice atoms reduced by the losses for electronic stopping of atoms in the displacement cascade. E_d is the effective threshold displacement energy equal to 40 eV for all materials considered here, and T_i^{max} is the maximal kinetic energy of the primary knock on atoms produced in i-th reaction. Currently, IAEA nuclear data section database has provided the displacement cross-sections (ENDF/B format) evaluated by NRT and BCA-MD models, and **Figure 1-3** show these cross-sections for Cr, Fe, and Zr nuclides with incident proton beam. As shown in the figures, the difference between the nuclear data from two models is gradually increased over about 3 keV, and the data produced from new model are generally lower than the other.

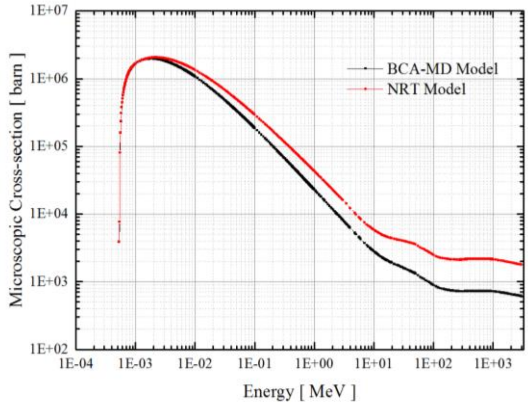
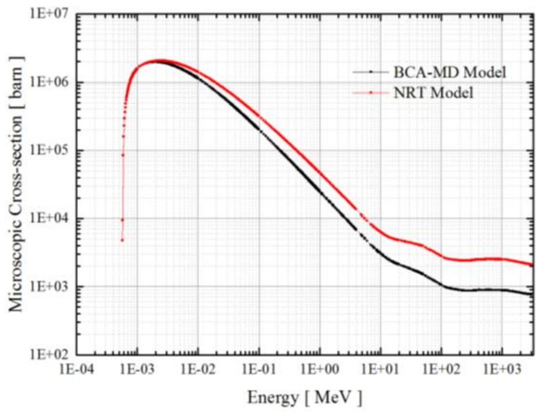


Figure 1. Displacement Cross-section for Cr Nuclide



(b) Fe

Figure 2. Displacement Cross-section for Fe Nuclide

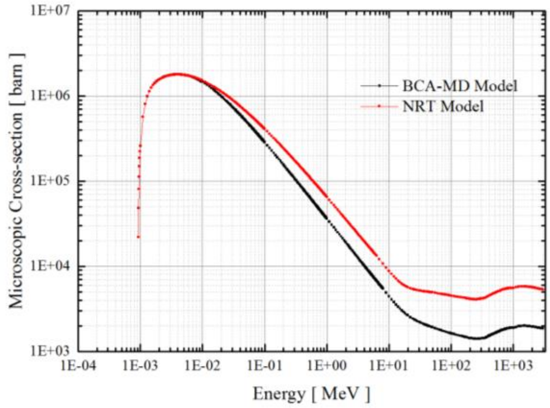


Figure 3. Displacement Cross-section for Zr Nuclide

The DPA calculation is performed by using displacement cross-section with incident radiation spectrum, and the general expression for the evaluation can be written as **Eq. (3)**;

$$DPA = \int \sigma_d(E) \times \frac{d\phi(E)}{dE} dE \qquad (3)$$

where $\varphi(E)$ is the radiation fluence (particles/cm^2) of which energy spectrum is calculated by MCNPX 2.7.0 code. Also, the calculation condition is assumed to be irradiated by 11 MeV proton beam on Zir-4 specimen of 0.6mm thickness.

3. Results and Discussions

Figure 4 shows the deposited energy distribution of 11 MeV proton beam in the Zir-4 specimen. The deposited energy is continually increased along the track of incident proton beam, and its bragg peak is shown at the point of about 0.44mm thickness. It is confirm that the sum of deposited energy in the specimen is same with the energy of incident proton beam. In **Figure 5**, the proton induced material damage is evaluated using the displacement cross-sections based on NRT and BCA-MD models, which is the results for a proton particle. The trend of DPA distribution is similar

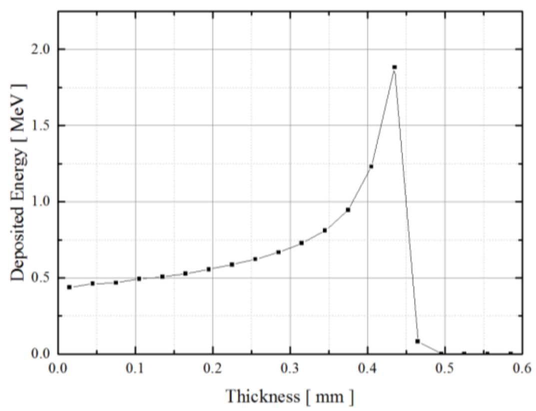


Figure 4. Deposited Energy Distribution of Incident Proton Beam Along to the Depth of Zir-4 Specimen

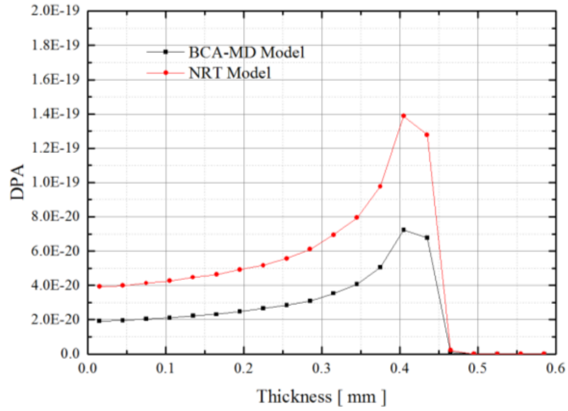


Figure 5. Material Damage Distribution from Incident Proton Beam Along to the Depth of Zir-4 Specimen

with the deposited energy distribution of incident proton beam, but the maximum DPA value is shown at the point of about 0.41mm thickness. Also, it is shown that the result using the cross-section based on BCA-MD model is lower about 2 times than the other.

4. Conclusions

The proton induced material damage is evaluated by using the displacement cross-sections, and the effect of nuclear data on the evaluation is specifically analyzed with MCNPX code. First, there is significant difference between the nuclear data from existing and new models, and the new evaluated data is generally lower than the existing one. Second, the position of maximum DPA is slightly differed with the position of maximum energy deposition, and the evaluation using new evaluated data is lower about 2 times than the other. Hence, it seems that the evaluation for neutron induced material damage is also need by using the above-mentioned method.

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