Calculation of athermal recombination corrected dpa cross sections for proton, deuteron and heavy-ion irradiations using the PHITS code

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Abstract. To provide the athermal recombination corrected dpa (arc-dpa) cross sections for proton, deuteron and heavy ion irradiations in the energy range from 1 MeV/u to 3 GeV/u., the defect production efficiencies for aluminium, copper and tungsten were implemented in the radiation damage model in PHITS. In general, the dpa cross section is large with increasing the number of protons of incident particle. For high-energy (around 1 GeV/u) proton and deuteron irradiation, the dpa cross section is close to that under ^{12}C irradiation due to secondaries produced by the nuclear reaction. The ratio of arc-dpa cross section to the conventional Norgett-Robinson-Torrens dpa (NRT-dpa) cross section is around 0.2 with incident energies over 100 MeV for proton and deuteron irradiations. For the case of ^{12}C and ^{48}Ca, this ratio is ranged from 0.3 to 0.4 for incident beam energies below 3 GeV/u.

1 Introduction

The displacement damage calculation method in the Particle and Heavy Ion Transport code System (PHITS) [1] has been developed using the screened Coulomb scattering to evaluate the energy of the target Primary Knock on Atom (PKA) created by the projectile and the "secondary particles" which include all particles created from the sequential nuclear reactions [1]. This method enables us to calculate displacement cross sections of materials for various particle such as proton, deuteron and heavy-ion in the wide energy range. To calculate the number of displaced atoms, the conventional Norgett-Robinson-Torrens (NRT) model [2] has been widely used. Recently, K. Nordlund et al. provided the athermal recombination corrected (arc) displacement per atom (dpa) function obtained from MD simulations providing more physically realistic descriptions of primary defect creation in materials [3]. Therefore, the arc-dpa will be used for efficient predictions of the usable lifetime of materials in various accelerator facilities with proton, deuteron and heavy ion beams.

To provide the arc-dpa cross sections of aluinum, copper and tungsten for proton, deuteron and heavy-ion irradiations, the arc-dpa function related with the defect production efficiency was implemented in the radiation damage model in PHITS [4, 5]. The parameters included in the arc-dpa function were taken from the paper [3, 6]. For the displacement cross sections of copper under proton irradiations with the energy range between 100 MeV and 3 GeV, we found that the NRT-dpa cross sections are larger than the arc-dpa cross sections by a factor of ~3 and the arc-dpa cross sections using PHITS give good agreements with the experimental data [7].

In this paper, we calculated the arc-dpa cross sections of the selected materials (aluminium, copper and tungsten) for proton, deuteron and heavy-ion (^{12}C and ^{40}Ca) irradiations in the high-energy region between 100 MeV/u and 3 GeV/u and compare them with the NRT-dpa cross sections for discussions about particle and material dependencies of the athermal recombination correction.

2 Displacement damage calculation method with PHITS

There are two parts for displacement calculation using PHITS [4, 5]. One is Coulomb elastic scattering cross section between incident particles and target atom. The NRT-dpa cross section is obtained by integral between Coulomb elastic scattering cross sections and the number of atomic displacements. Another is nuclear reaction including elastic and in-elastic scattering with nucleus. In this section, we will show overview of the calculation method. Details for the displacement damage calculation method were in our previous paper [4].

The number of displacement atoms using NRT model is shown as below:

$$N_{\mathrm{NRT}} = \frac{0.8}{2E_{\mathrm{D}}} E_{\mathrm{d}} \qquad (1)$$

where E_{d} is the damage energy transferred to lattice atoms and E_{D} is the threshold displacement energy. The NRT-dpa cross sections for the incident charged particle and the target atom is obtained by using the following equation:

$$\sigma_{\mathrm{NRT}} = \int_{t_{\mathrm{d}}}^{t_{\max}} d\sigma_{\mathrm{sc}}/dt \cdot N_{\mathrm{NRT}}(t)\, dt \qquad (2)$$

where t is the dimensionless collision parameter including information of the kinetic energy of recoil. The $t_{\max}$, maximum kinetic energy of recoil, is determined by the

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kinematics between incident charged particle and target atom. T_d is the dimension less energy of the threshold displacement energy E_D. $d\sigma_{sc}/dt$ is the Coulomb elastic scattering cross section.

In the energy range of incident particle above 10 MeV/u, secondaries are produced by nuclear reactions. In this work, the NRT dpa cross section of secondaries were obtained by the Monte Carlo calculation of charged particles incident reactions on a thin sample. It is obtained by the following equation:

$$\sigma_{\mathrm{NRT}} = \frac{DPA}{\phi} = \frac{\sum_{i=1}^{N} N_{NRT\,i}}{n_0 A} / \phi \qquad (3)$$

where n_0 is the Avogadro number of a target and A is the atomic number of a target. i denotes the ith of secondaries produced by nuclear reaction. N_{NRT} is calculated by Eq. (1) for event-by-event. The damage energy transferred to lattice atoms in Eq. (1) is obtained by the kinetic energy of secondaries produced by the direct model and the static model. For the direct process, INCL-4 model [8] and the JQMD model [9] is used for nucleon and heavy-ion, respectively. The GEM model [10] is employed for the static process of nuclear reactions. The geometry of a target was a cylinder with 10 mm diameter and 1 μm thickness and that of a beam was a circle with 10 mm diameter. In the calculations, the kinetic energies of secondaries are scored when secondaries are produced in a sample. ϕ is a beam fluence on a target.

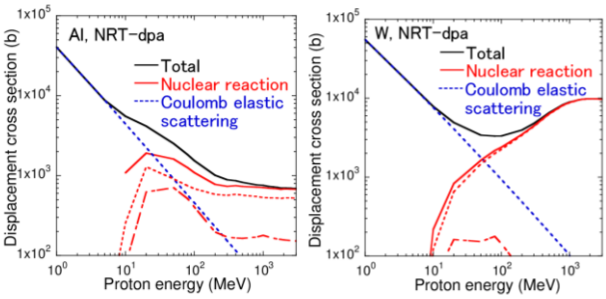

Figure 1. NRT-dpa cross sections for proton irradiation on aluminium and tungsten.

Figure 1 shows the NRT-dpa cross sections for proton irradiation on aluminium and tungsten. Solid red line is cross section obtained by secondaries produce by nuclear reactions with Eq. (2). Dashed line is component of dpa cross section produced by incident charged particles with Eq. (1). Contribution of nuclear reaction is dominant in the energy region above 10 MeV because the nuclear reaction cross section related with the number of secondary particles increases with proton energy. For the comparison between aluminum and tungsten in the energy region above 100 MeV, displacement cross section of tungsten increases with proton energy and that of aluminum is nearly constant. This is because that the damage energy, E_d, in Eq. (1) increases with recoil energy produced by proton-tungsten nuclear reactions. On the other hand, E_d is close to constant with increasing recoil energy for the proton-aluminum nuclear reaction.

Figure 2 shows the NRT-dpa cross sections for ^{48}Ca irradiation on aluminium and tungsten. For the comparison with proton irradiation, the Coulomb scattering between ^{48}Ca and a target is dominant in the energy region above 10 MeV/u. This trend is strong with increasing the number of protons for the incident beam.

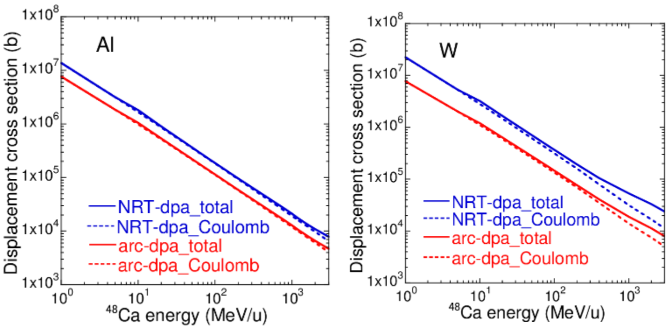

Figure 2. NRT-dpa cross sections for ^{48}Ca irradiation on aluminium and tungsten.

The arc-dpa cross section was calculated using the displacement efficiency function ζ obtained by the molecular dynamics (MD) simulation study [3].

$$N_{\mathrm{arc}} = \frac{0.8}{2E_{\mathrm{D}}} E_{\mathrm{d}} \zeta(E_{\mathrm{d}}) \qquad (4)$$

$$\zeta(\mathrm{E}_d) = \frac{1-c}{(2E_D/0.8)^b} {E_d}^b + \mathrm{c} \qquad (5)$$

where b and c are the tabulated parameters for each nucleus obtained by the Molecular study [3]. Fig. 2 shows the defect production efficiency ζ of aluminium, copper and tungsten to the nuclear damage energy. The numerical values of b and c were given by Nordlund et al. for copper and tungsten [3] and Konobeyev et al. [6] for aluminum in Fig. 2. E_D for aluminium, copper and tungsten was 27 eV, 33 eV and 70 eV, respectively. As damage energy increases, efficiency steadily decreases to a value of 0.2 for 10 keV damage energy in tungsten and copper. In the damage energy region above 10 keV, the damage efficiency was adopted as constant value because the MD simulation study [3] was carried out at damage energy below 10 keV. The arc-dpa cross sections are calculated with Eq. (2) for incident charged particles and Eq. (3) for secondaries produced by nuclear reactions using Narc in Eq. (4), respectively.

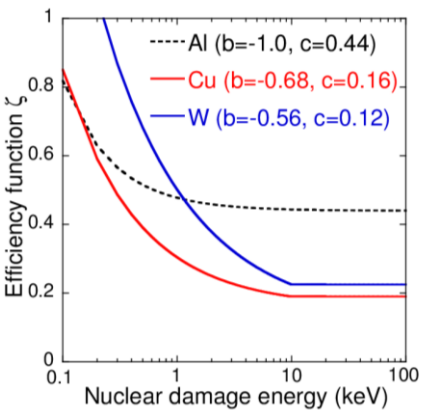

Figure 3. Defect production efficiency of aluminium, copper and tungsten

3 arc-dpa cross sections for proton, deuteron, ^{12}C and ^{48}Ca irradiations

Figure 4 shows arc-dpa cross sections of aluminium, copper and tungsten for proton, deuteron, ^{12}C and ^{40}Ca beam irradiation in the energy range from 1 MeV/u to 3 GeV/u. In general, dpa cross section is large with increasing the number of protons of incident particle. For high-energy (around 1 GeV/u) proton or deuteron irradiation, dpa value is close to that under ^{12}C irradiation due to secondaries produced by the nuclear reaction.

Figure 5 shows the ratio of arc-dpa cross section to NRT-dpa cross section for proton, deuteron, ^{12}C and ^{48}Ca irradiations. This ratio is related with defect production efficiencies in Fig. 3. For proton and deuteron irradiations, the ratio is around 0.2 with incident energies over 100 MeV because damage efficiency is also around 0.2 with damage energies above 10 keV. For the case of ^{12}C and ^{48}Ca, this ratio is ranged from 0.3 to 0.4 because damage energies are around several keV for incident beam energies below 3 GeV/u.

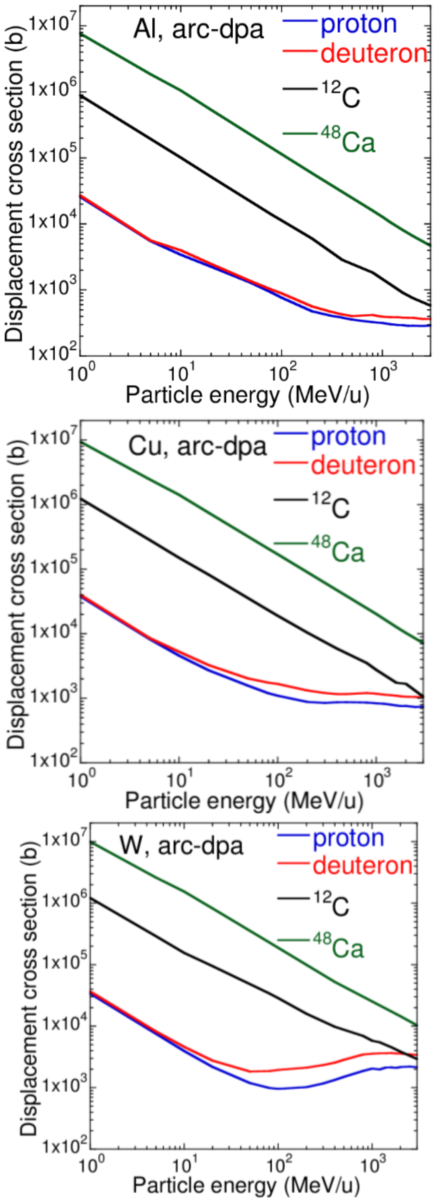

Figure 4. arc-dpa cross sections for proton, deuteron, ^{12}C and ^{48}Ca irradiations

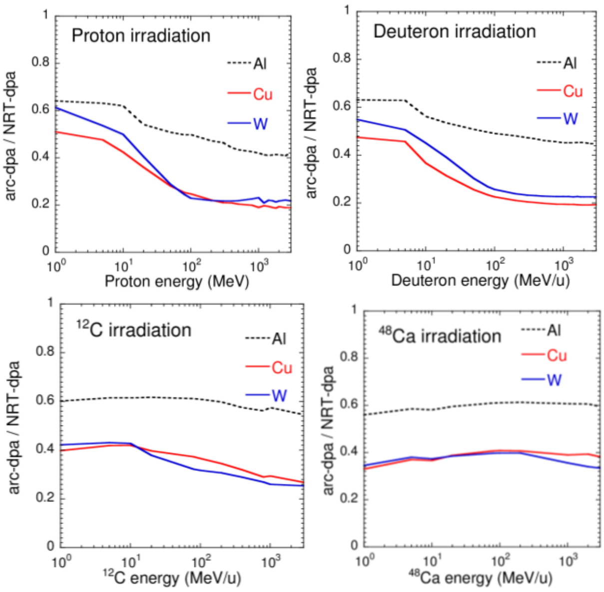

Figure 5. arc-dpa cross sections for proton, deuteron, ^{12}C and ^{48}Ca irradiations

4 Summary

To provide the arc-dpa cross sections for proton, deuteron and heavy ion irradiations in the energy range from 1 MeV/u to 3 GeV/u., the defect production efficiencies for aluminium, copper and tungsten were implemented in the radiation damage model in PHITS. The parameters included in the defect production efficiencies were taken from the paper written by K. Nordlund et al. for copper and tungsten and Konobeyev for aluminium. In general, dpa is large with increasing the number of protons of incident particle. For high-energy (around 1 GeV/u) proton and deuteron irradiation, dpa value is close to that under ^{12}C irradiation due to secondaries produced by the nuclear reaction. The ratio of arc-dpa cross section to NRT-dpa cross section is around 0.2 with incident energies over 100 MeV for proton and deuteron irradiations. For the case of ^{12}C and ^{48}Ca, this ratio is ranged from 0.3 to 0.4 for incident beam energies below 3 GeV/u.

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