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Implementing displacement damage calculations for electrons and gamma rays in the Particle and Heavy-Ion Transport code System

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ABSTRACT

In this study, the Monte Carlo displacement damage calculation method in the Particle and Heavy-Ion Transport code System (PHITS) was improved to calculate displacements per atom (DPA) values due to irradiation by electrons (or positrons) and gamma rays. For the damage due to electrons and gamma rays, PHITS simulates electromagnetic cascades using the Electron Gamma Shower version 5 (EGS5) algorithm and calculates DPA values using the recoil energies and the McKinley–Feshbach cross section. A comparison of DPA values calculated by PHITS and the Monte Carlo assisted Classical Method (MCCM) reveals that they were in good agreement for gamma-ray irradiations of silicon and iron at energies that were less than 10 MeV. Above 10 MeV, PHITS can calculate DPA values not only for electrons but also for charged particles produced by photonuclear reactions. In DPA depth distributions under electron and gamma-ray irradiations, build-up effects can be observed near the target's surface. For irradiation of 90-cm-thick carbon by protons with energies of more than 30 GeV, the ratio of the secondary electron DPA values to the total DPA values is more than 10% and increases with an increase in incident energy. In summary, PHITS can calculate DPA values for all particles and materials over a wide energy range between 1 keV and 1 TeV for electrons, gamma rays, and charged particles and between 10^{-5} eV and 1 TeV for neutrons.

1. Introduction

Displacement damage from electrons (or positrons) is important both in electron microscopes for radiation damage studies and in target materials at electron accelerator facilities for clinical treatments that involve X-ray and electron radiotherapy. Owing to the electron's low mass, electrons with sufficient energy (>100 keV) that can impart ~ 10 eV to a nucleus in an electron-nucleus collision are relativistic and cause lattice atom displacements [1]. The high flux isotope reactor has also reported that gamma-ray radiation damage to reactor core materials is important [2].

Secondary electrons produced by gamma-ray-induced reactions can also displace atoms. At proton accelerator facilities with energies above ~ 1 GeV, such as J-PARC [3] with ~ 50 GeV protons and CERN [4] with ~ 400 GeV protons, many types of particles are produced by spallation reactions, including gamma rays and electrons. Estimating the radiation damage at such accelerator facilities is important not only for neutrons and charged particles but also for electrons and gamma rays.

The number of displacements per atom (DPA) is a reference value that is used to characterize and compare the radiation damage induced in crystalline materials by projectiles such as neutrons at fission, fusion, and accelerator facilities. In a previous study, researchers have developed a method [5,6] for calculating DPA values for materials with arbitrary geometries that are being irradiated with neutrons, charged particles, and mesons using the event generator in the Particle and Heavy-Ion Transport code System (PHITS) [7]. These PHITS-based DPA calculations use event-by-event analysis of the recoil energies and displacement cross sections of all the particles, except for electrons and gamma rays, using the event generator with a wide energy range from 1 keV to 1 TeV for charged particles and from 10^{-5} eV to 1 TeV for neutrons [4]. However, other particle transport codes, such as MARS [8] and FLUKA [9], use the displacement cross-section database derived by the NJOY nuclear data processing system code [10] for neutrons and intra-nuclear cascade models [8,9] for high-energy particles.

For DPA calculations involving electrons and gamma rays, the Monte Carlo-based Electron Gamma Shower version 4 (EGS4) user code called UCDPA [11] has been used to conduct Monte Carlo simulations of DPA depth distributions for electrons and gamma rays from 1 to 10 MeV. The Monte Carlo assisted Classical Method (MCCM) [12], which relates established atom displacement theories to the electron and gamma-ray secondary fluence distributions calculated by the Monte Carlo N-Particle Transport code, has also been adopted to estimate DPA values for electron and gamma-ray irradiations.

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In this study, we calculate DPA values for all particles (not only neutrons, charged particles, and mesons but also electrons and gamma rays) and materials in a wide energy range using PHITS. To do this, a method for calculating the displacement damage due to electron and gamma-ray irradiation in PHITS by considering electromagnetic cascades using the EGS5 algorithm has been implemented [13]. Three years ago, the EGS5 algorithm was incorporated into PHITS to generate electron and gamma-ray events. The benchmark calculations of the electron bremsstrahlung and transmission and absorption of electrons using the EGS5 mode have already confirmed that the experimental data and calculated results are in good agreement [14]. The McKinley–Feshbach cross section [1,15,16], which is the relativistic and quantum mechanical cross section for recoil under electron irradiation, is adopted for the electron displacement damage calculation.

We also present the following applications of displacement damage calculations using PHITS: (1) DPA depth distributions in 10-cm-thick metals under gamma-ray irradiation; (2) DPA depth distributions in 1-cm-thick metals under electron irradiation; and (3) DPA depth distributions for electrons in 90-cm-thick graphite under high-energy proton irradiation at energies between 3 and 400 GeV.

2. Radiation damage model for electrons, positrons, and gamma rays implemented in PHITS

Fig. 1 summarizes the physics models that are used in PHITS to simulate nuclear and atomic collisions [14]. The important point is that the recoil and secondary charged particles generate atomic cascade damage via Coulomb scattering. For neutron irradiations at energies less than 20 MeV, the recoil particles are created by the event generator for each event [17,18]. For high-energy neutron and charged particle irradiations, the recoil and secondary particles produced by nuclear reactions are calculated using INCL4.6 [19] in the energy range of 20 MeV to 3 GeV, and by JAM [20] from 3 GeV to 1 TeV. Further details of the DPA calculations for neutrons and charged particles have been mentioned in previous studies [5,6].

For electron and gamma-ray irradiations, the EGS5 algorithm is used for electromagnetic cascades across a wide energy range of 1 keV to 1 TeV. When metals are irradiated by gamma rays above a few hundred keV, their atoms collide with energetic electrons produced by Compton scattering or pair creation. As the binding energies of atoms in the metal lattice, which are called the displacement energies, are between 20 and 90 eV and the ratios between the electron and metal atom masses are $\sim 10^5$, electrons above 400 keV can remove an atom from the lattice [11]. The maximum kinetic energy $T_{\max}$ of the recoil atom is calculated as follows:

$$T_{max} = 2\frac{m}{M}\frac{(E+2mc^2)E}{mc^2}, \tag{1}$$

where m is the electron's mass, M is the target atom's mass, c is the speed of light, and E is the electron's kinetic energy. The scattering of electrons by unscreened target atomic nuclei of charge number Z was investigated by Mott [21,22], who derived the differential cross section. McKinley and Feshbach [15,16] derived the relativistic and quantum mechanical cross section using Mott's differential cross section as follows:

$$\sigma_{McF} = \frac{4\pi a_0^2 Z^2 E_R^2}{m^2c^4\beta^4\gamma^2}\left[\left(\frac{T_{max}}{E_d}-1\right)-\beta^2 ln\frac{T_{max}}{E_d} + \pi\alpha\beta\left\{2\left[\left(\frac{T_{max}}{E_d}\right)^{1/2}-1\right]-ln\frac{T_{max}}{E_d}\right\}\right], \tag{2}$$

where a_0 is the Bohr radius, E_R is the Rydberg energy, β is the ratio of the electron and light velocities, $e^2/2a_0 = 13.6$ eV, and $\alpha = Z/137$. If the recoil atom's kinetic energy is greater than the displacement energy, it can dislocate secondary atoms and remove them from the lattice. The displacement cross section is calculated using the number of secondary displaced atoms υ(T) as follows:

$$\sigma_{damage} = \sigma_{McF}\,\upsilon(\mathrm{T}) = \sigma_{McF}\frac{T}{2E_d}, \tag{3}$$

where T is the recoil kinetic energy and E_d is the displacement threshold energy used in PHITS [6]. As the EGS5 algorithm cannot calculate the kinetic energies of recoil particles irradiated with electrons, the mean recoil energy $\overline{T}$ is obtained as follows:

$$\overline{T} = \frac{\int_{E_d}^{T_{max}} T\frac{d\sigma}{dT}dT}{\int_{E_d}^{T_{max}} \frac{d\sigma}{dT}dT}, \tag{4}$$

where $d\sigma/dT$, the differential scattering cross section for Coulomb scattering [15,16], is written in terms of T and T_{max} as follows:

$$d\sigma/dT = \frac{4\pi a_0^2 Z^2 E_R^2}{m^2c^4\beta^4\gamma^2}\left\{1-\beta^2\frac{T}{T_{max}} + \pi\alpha\beta\left\{\left(\frac{T}{T_{max}}\right)^{1/2} - \frac{T}{T_{max}}\right\}\right\}\frac{T_{max}}{T^2}. \tag{5}$$

For irradiation by gamma rays with energies above 20 MeV, protons, neutrons, charged particles, and recoil particles are produced by photonuclear reactions [23], as shown in Fig. 1. Further details of the displacement damage calculations for charged particles are given in previous studies [5,6].

Fig. 2 shows the energy dependence of the fluence-normalized DPA values for 3 × 3 × 3 cm^3 silicon and iron blocks. MCCM results from [12] are also shown for comparison with the PHITS results. Below 10 MeV, the DPA values from PHITS and MCCM are in good agreement for silicon and iron. Above 10 MeV, the DPA values include not only secondary electrons but also charged and recoil particles produced by

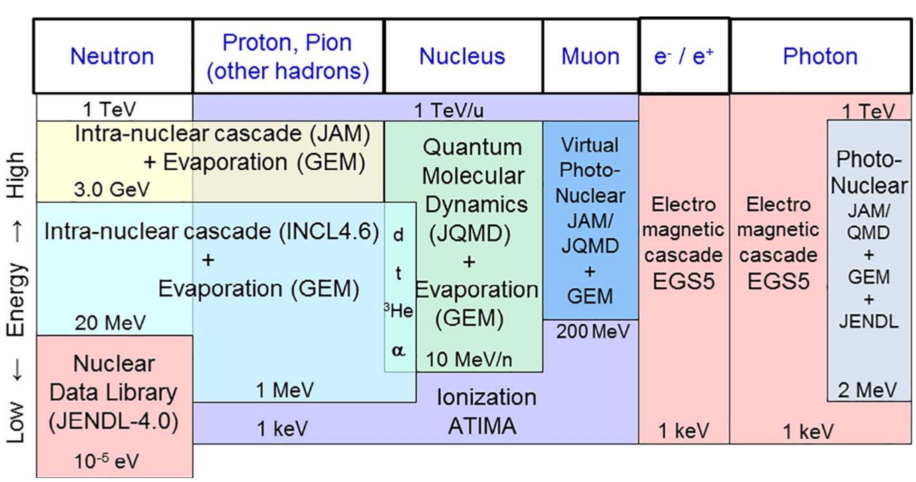

Fig. 1. Physics models recommended for use in PHITS to simulate nuclear and atomic collisions [14].