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Application of EGS4 for Evaluation of Material Damage due to Gamma-ray Irradiation

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Abstract

An EGS4 user code named UCDPA was developed for the simulation of material damages by the electrons and photons considering electromagnetic cascade. The calculated depth distributions of dpa in iron slab were compared to the measurements of material hardening due to 2 and 2.5MeV electron beam irradiations. The calculated dpa distributions and the measured hardening distributions were in a similar shape which have a peak at about 0.2mm from irradiated surface. The depth distributions of dpa were also calculated for photons from 0.7 to 10 MeV.

1 Introduction

The unexpected acceleration of radiation-induced embrittlement was discovered in the surveillance materials of High Flux Isotope Reactor (HFIR) in 1986[1]. A lot of studies have been made to explain this phenomena, and the gamma-ray induced reactions were supposed to be the dominant process[2],[3]. Because the energy required to displace atoms from metallic lattice (Lindhard cutoff energy ; Ed) is few ten eV, the electrons produced from gamma-ray can knock-on the atoms when the electron energy is above several hundred keV. In preceding studies, the material damages due to gamma rays have been evaluated with the primary knock-on atom (PKA) or displacement per atom (dpa) cross sections for photons and photon flux in materials. These damage cross sections have been calculated assuming the secondary electron spectrum in infinite media of metals, therefore the damage distributions in depth of materials were not considered. These studies also have not been considered the contribution of electrons produced at deep position by bremsstrahlang photons.

We developed an user code for EGS4[4] named UCDPA for the simulation of material damages by the electrons and photons considering electromagnetic cascade. The user code calculates the PKA and dpa cross sections of electrons with the kinetics of electron-atom collisions, and calculates damage distributions in a semi-infinite slab geometry. We calculated the dpa depth distributions in iron slab irradiated by 2 or 2.5MeV electrons and up to 10MeV photons with the user code.

2 Displacement Cross Sections

The mechanism of gamma-ray damage to metals is schematically shown in Fig.1. When the metal irradiated by gamma-rays above several hundreds keV, the atoms of metal suffer the collision with energitic electrons produced by compton scatterings or pair creations. Because the binding energy of atoms in metal lattice (displacement energy) is from 20eV to 40eV, and mass ratios of electron and metal atoms are about 10^5, the electrons above 400keV can remove an atom from the lattice. The removed atom is so called "Primary Knock-on Atom (PKA)". The PKA cross section, the number of

PKA's per unit fluence of electron, are calculated with following formula derived from Mott scattering cross section,

$$\begin{aligned}\sigma_P &= 4\pi\left(\frac{Za_0E_R}{mc^2}\right)^2 \\ &\cdot \frac{1}{\beta^4\gamma^2}\left[\left(\frac{T_m}{E_d}-1\right)\beta^2\ln\left(\frac{T_m}{E_d}\right)+\pi\alpha\beta\left\{2\left(\sqrt{\frac{T_m}{E_d}}-1\right)-\ln\left(\frac{T_m}{E_d}\right)\right\}\right]\end{aligned} \tag{1}$$

where,

Z :atomic number of target atom,

a_0 :Bohr radius ($= 0.529 \times 10^{-10}$m),

E_R :Rydberg energy : $e^2/2a_0 = 13.6$eV,

α $=Z/137$,

β :ratio of electron velocity to light velocity,

T_m $= 2\frac{m}{M}\frac{E}{mc^2}(E + 2mc^2)$ (maximum kinetic energy of recoil atom),

M :mass of target atom,

m :mass of electron,

E :electron kinetic energy,

E_d :displacement energy.

If the recoil atom has the kinetic energy above the displacement energy, secondary atoms can be knocked-on by PKA and removed from the lattice. The number of secondary displaced atoms per PKA of kinetic energy T is approximately calculated as follows,

$$\nu(T) = \begin{cases} 0, & T < E_d \\ 1, & E_d \leq T < 2E_d \\ \frac{T}{2E_d}, & 2E_d \leq T < L_C \\ \frac{L_C}{2E_d}, & T \geq L_C \end{cases} \tag{2}$$

The displacement per atom (dpa) cross section, total number of displaced atoms per unit fluence per a target atom, is calculated as $\sigma_P \cdot \nu(T)$. The calculated PKA and dpa cross sections are shown in Fig.2 for the displacement energy of 40eV.

3 UCDPA User Code

UCDPA is an EGS4 user code to calculate PKA and dpa by electrons or photons using Eq.(1) and (2). The target geometry is multi-layer, multi-lateral cylinder or multi-layer; semi-infinite slab. The irradiation condition is pencil beam or broad parallel beam of electron or photon. The PKA and dpa in each target layer and each lateral section are calculated by multiplying the electron track length with PKA or dpa cross sections in subroutine AUSGAB. The kinetic energy of PKA (T) used in Eq. (2) is assumed to be the average energy of recoil atom T_{av} obtained as follows.

$$\begin{aligned}\frac{T_{av}}{\sigma_P} &= 4\pi\left(\frac{Za_0E_R}{mc^2}\right)^2 \\ &\cdot \frac{1}{\beta^4\gamma^2}\left\{T_m - \ln\left(\frac{T_m}{E_d}\right) - \beta^2(T_m - E_d) + \pi\alpha\beta\cdot(T_m + E_d - 2\sqrt{T_m\cdot E_d})\right\}\end{aligned} \tag{3}$$

4 Electron Irradiation Experiment and Analysis

The UCDPA was applied to calculate the dpa distribution in a specimen of Fe-0.6wt%Cu alloy used for the experiment performed by JAERI[5] using 3MV single-ended electron accelerator of TIARA (JAERI-Takasaki). In this experiment, 5×10mm specimen was irradiated by 2MeV-10mA broad parallel beam of electrons. The specimen was heated to 250°C, and placed in vacuum. The difference of hardenings between irradiated (5-15 hours) and un-irradiated specimen (Δv) were measured.

The dpa and PKA distribution along the beam axis was calculated using UCDPA to compare the measured distribution of hardening. Fig.3 shows the calculated dpa and PKA distribution in an iron slab for electron energy of 2, 2.5 and 10MeV assuming that its displacement energy is 40eV. The dpa and PKA was same for the electron energy of 2MeV and 2.5MeV, because the kinetic energy of PKA was lower than displacement energy. The peak of dpa was observed at the depth of about 0.2mm from irradiated surface where the total number of primary and secondary electrons was maximum. The measured peak of hardening was also observed at the depth of few-hundred mm.

5 DPA Distribution From High Energy Photons

Depth distributions of dpa in an iron slab caused by photon irradiation were calculated for the photon energy from 700keV to 10MeV. In Fig.4 and Fig.5 are shown the calculated dpa distributions at depth from 0 to 10cm and the peak values of dpa at each photon energy, respectively. The peak of dpa appeared at more deep position and the width of peak became broader at the higher photon energy. The dpa decreases in exponential with depth at any photon energies. The peak value of dpa increases linearly with photon energy above 2MeV, and it increases in exponential below 2MeV.

6 Conclusion

UCDPA is a tool to evaluate the depth distribution of the material damage caused by gamma-ray or electron irradiation. The calculated dpa distributions showed that the peak of dpa is at the inside of materials. The detailed estimation of material damage in nuclear reactors, such as reactor vessels, shrouds, or other structures, can be performed by the combination of the neutron-gamma coupled shielding calculations and gamma-ray damage calculations with UCDPA.

References

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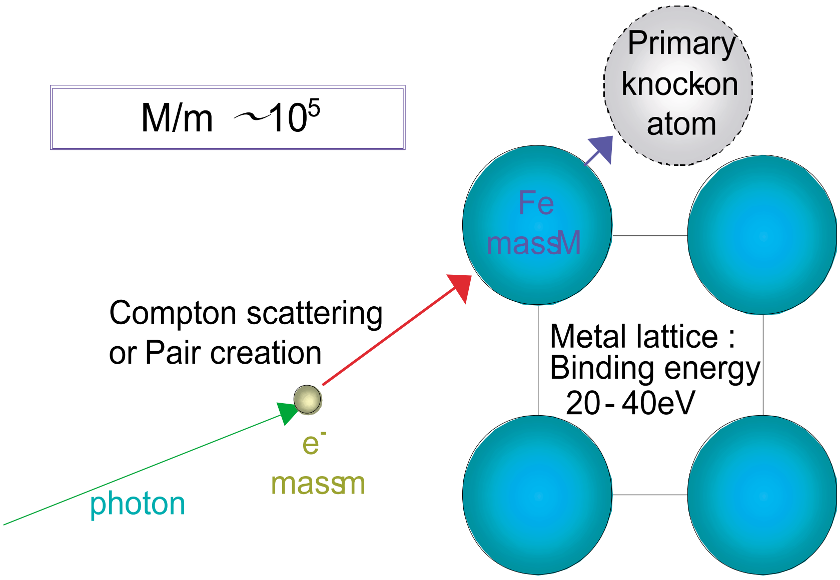

Figure 1: Schematic mechanism of material damage caused by gamma-ray irradiation.

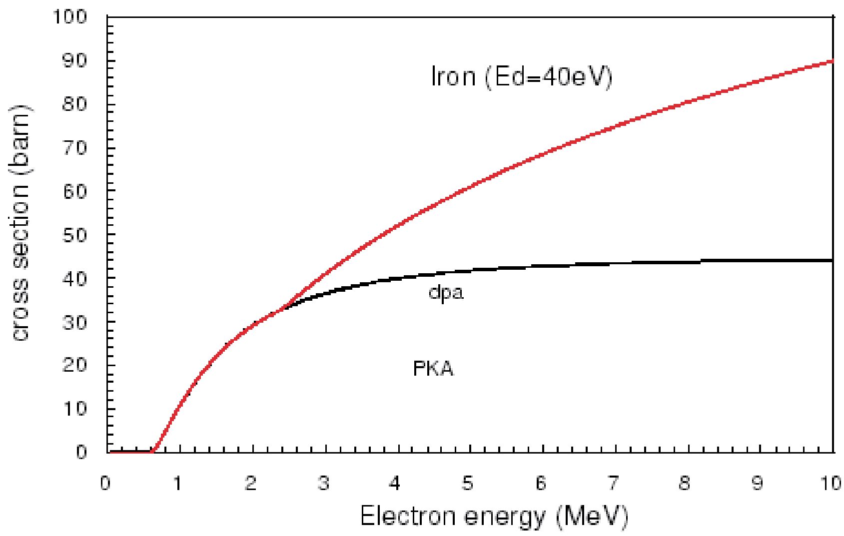

Figure 2: Calculated PKA and dpa cross sections of iron for electrons. Displacement energy (Ed) is assumed to be 40eV.

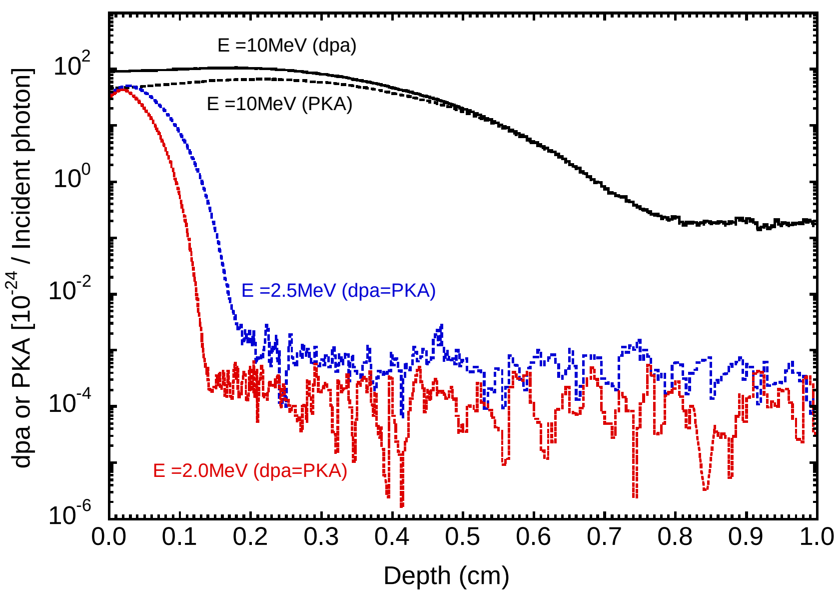

Figure 3: Calculated depth distribution of dpa in iron slab irradiated by 2.0, 2.5 and 10MeV broad parallel electron beam. The fluctuations at deep position are due to statistical errors of Monte Carlo calculations.

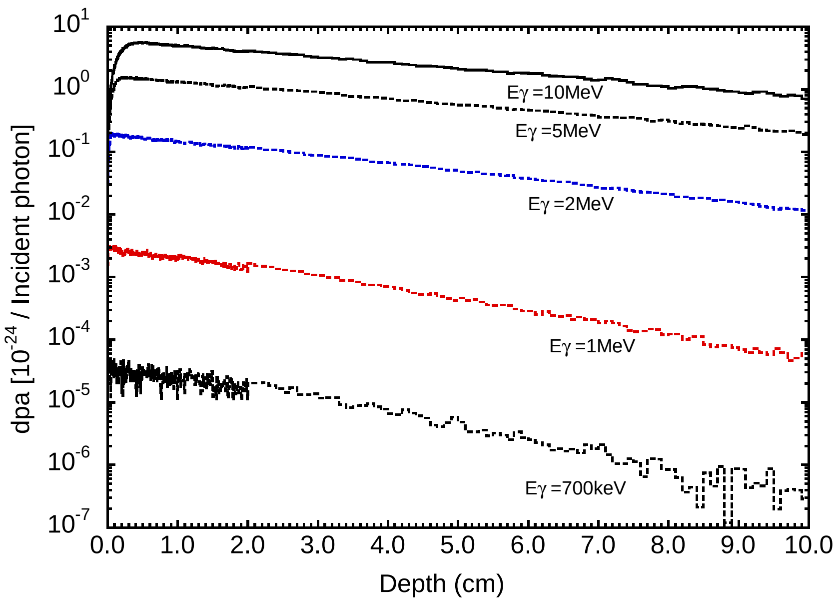

Figure 4: Calculated depth distribution of dpa in iron slab irradiated by 700keV - 10MeV broad parallel photon beam. The fluctuations for lower photon energies are due to statistical errors of Monte Carlo calculations.

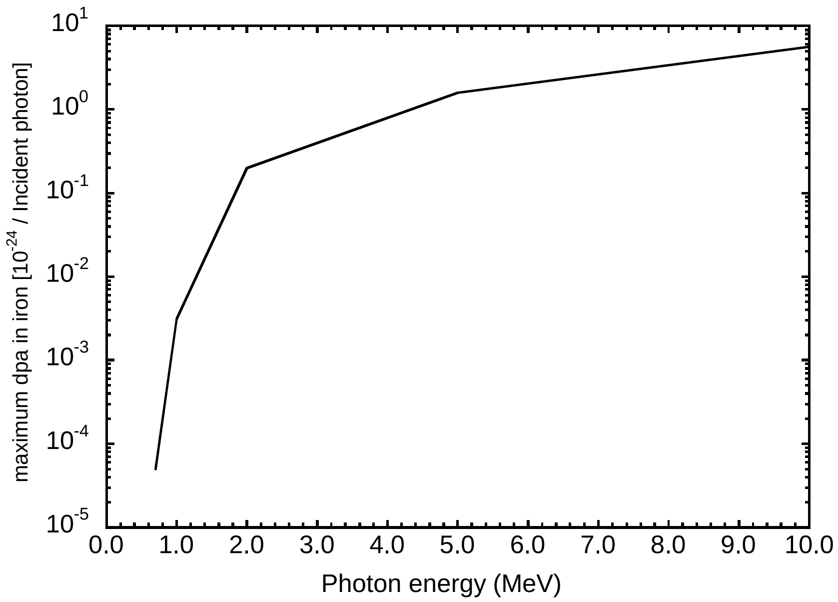

Figure 5: Maximum dpa in iron slab irradiated by 700keV - 10MeV photons.