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Improved calculation of displacements per atom cross section in solids by gamma and electron irradiation

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ABSTRACT

Several authors had estimated the displacements per atom cross sections under different approximations and models, including most of the main gamma- and electron-material interaction processes. These previous works used numerical approximation formulas which are applicable for limited energy ranges. We proposed the Monte Carlo assisted Classical Method (MCCM), which relates the established theories about atom displacements to the electron and positron secondary fluence distributions calculated from the Monte Carlo simulation. In this study the MCCM procedure is adapted in order to estimate the displacements per atom cross sections for gamma and electron irradiation. The results obtained through this procedure are compared with previous theoretical calculations. An improvement in about 10–90% for the gamma irradiation induced dpa cross section is observed in our results on regard to the previous evaluations for the studied incident energies. On the other hand, the dpa cross section values produced by irradiation with electrons are improved by our calculations in about 5–50% when compared with the theoretical approximations. When thin samples are irradiated with electrons, more precise results are obtained through the MCCM (in about 20–70%) with respect to the previous studies.

1. Introduction

The issue of damage caused by different radiation sources in different materials has been and is still widely discussed by the scientific community. This topic is of great importance involving the changes they may induce in the properties of those materials. The primary event and one of the most important processes related with this radiation damage is the production of atom displacements, which first step is the generation of a primary knock-on atom (PKA), with kinetic energy T. If this interaction can be described through a differential cross section $d\sigma(E,T)/dT$, then for an incident radiation with energy E, which fluence is $\Phi(E)$, the total number of primary atoms per unit volume is:

$$N_T = N_a \int_{T_d}^{T_{\max}} \int_{E_c}^{E_{\max}} \frac{d\sigma(E,T)}{dT} \Phi(E)\, dE\, dT, \tag{1}$$

where N_a is the number of atoms per unit volume, T_d is the minimum energy an atom needs to be displaced, $T_{\max}$ is the maximum energy of the recoil atoms, E_c is the lowest radiation energy which can transfer energy T_d to a lattice atom and $E_{\max}$ is the maximum energy of the radiation spectrum.

Thus, for a monoenergetic incident fluence, it is possible to evaluate the total number of primaries per unit volume as:

$$N_T = N_a \Phi_0 \sigma(E_0, T_d), \tag{2}$$

being E_0 the energy of the incident radiation fluence Φ_0 and $\sigma(E_0, T_d)$ could be seen as the total atom displacement cross section. Therefore, the point is to find the adequate cross section for each case under study. However, there are no tools or methods for an accurate determination of such cross section for atom displacements determination in the case of electron and gamma irradiation at present.

In the late 1950's Oen and Holmes [1] and Cahn [2] proposed a methodology to calculate the atom displacements cross section in solids produced by gamma rays. In the last two decades several updated procedures for atom displacements cross section estimations have been proposed [3–7]. However, all those calculations have a restricted character and meaning, as will discussed in next section.

In a previous work [8] we presented an alternative approach to calculate the atom displacements distributions in high

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temperature superconductors involving gamma radiation interactions and transport properties. Later, the contribution from positrons was also included in these studies [9], introducing a calculation procedure for atom displacements estimations [10].

Within this framework, this manuscript presents an improved methodology for the calculation of atom displacements cross section in solids by gamma rays and electrons irradiation. The results from previous mentioned theoretical calculations are then compared and analyzed with those obtained with our proposal.

2. Previous calculation procedures

Gamma radiation produces atom displacements through secondary electrons and positrons. The calculation of the differential cross section is thus complex, since involves different intermediate processes. Each of these processes may be dominant for a given energy and a given target material. Oen and Holmes [1] proposed a methodology to calculate displacement cross sections in solids by gamma rays. Cahn [2] also applied this methodology to calculate the total number of displaced atoms in germanium and silicon due to electrons and gamma rays of energies up to 7 MeV.

Following their idea, the true cross section in this case may be expressed formally by adding up all gamma-material interaction cross sections for the various mechanisms for energy transfer from primary gamma radiation to secondary electrons. For these processes, the intermediate electron behavior details in the lattice must be considered. Since one of the principal experimental advantages of gamma rays is near uniformity of damage production over large samples, it is felt that the most useful calculation considers the entire range of the electron as falling within the specimen. Thus, one additional result is the "thick target" cross sections for atom displacement by electrons.

Therefore, it is assumed that the energetic electrons produced by the gamma rays are stopped inside the solid sample. The average number of displaced atoms produced by an electron over its path, $\overline{n}(E_0)$, is thus found by integrating the elastic electron–atom interaction cross section over the electron range, also known as the displacements cross section $\sigma_d(E)$, obtaining:

$$\overline{n}(E_0) = N_a \int_0^{E_0} \frac{\sigma_d(E)}{(-\mathrm{d}E/\mathrm{d}x)}\, dE, \tag{3}$$

where $(-\mathrm{d}E/\mathrm{d}x)$ represents the electron energy change with respect to the electron path [11]. The elastic electron–atom interaction cross section is discussed in details in the next section.

For the gamma-material interaction cross sections Oen and Holmes considered Compton scattering with the assumption of single displacement for the primary recoiled atom. Cahn considers the main three processes of gamma interaction with matter producing secondary electrons: Compton scattering, photoeffect and pair production. In the last two decades several updated cross sections have been proposed.

The calculation by Baumann [3] was based on Oen's electron-induced displacement cross section [12] with the displacement energies of 28 eV and 40 eV, considering Compton scattering and pair production. Alexander and Rehn [13] carried out their calculation considering all three gamma-material interactions with the McKinley–Feshbach approximation for electron-induced displacement [14]. Kwon and Motta [5] proposed atom displacements cross sections for various metals, considering three gamma-material interactions and using Oen's electron-induced displacement cross section with the displacement energies of 24 eV and 40 eV. The contribution of positrons produced from the pair production was neglected in Kwon–Motta's calculation and was treated as electrons's in Baumann's and Alexander–Rehn's calculations.

Fukuya and Kimura [7] calculated gamma-induced atom displacements cross sections of iron considering all three gamma-material interactions with the McKinley–Feshbach approximation for electron-induced displacement and displacement energies of 25 eV and 40 eV. They took into account both electron and positron-induced displacements by separate.

All these calculations have a restricted character. They follow the Oen–Holmes–Cahn calculation procedure, which does not take into account the cascade process of the showering of gamma rays and the secondary electron and positron, occurring during radiation transport inside materials. They neither can obtain the volume distribution of atom displacements damage inside the material.

3. The Monte Carlo assisted Classical Method

The proposed Monte Carlo assisted Classical Method (MCCM) relates the Oen–Holmes and Cahn established theories [1,2] (here on referred as "classical theories") about atom displacements to the electron and positron fluence distributions calculated from the Monte Carlo simulation.

The proposal mainly consists in replacing the analytical distributions of particles produced in gamma and electron interactions with material by those obtained through the Monte Carlo simulation of radiation transport in matter. That is, defining the total number of atom displacements (AD) per volume unit as:

$$N_{\mathrm{AD}} = \frac{1}{V} \int_0^{E_0} \overline{n}(E) N_e(E)\, dE, \tag{4}$$

where V is the studied volume, $\overline{n}(E)$ is given by Eq. (3), and $N_e(E)$ is the energy distribution of secondary particles calculated by Monte Carlo simulation in the volume V. The code system used for simulation purposes (described in Section 3.2) allows to obtain the average energy fluence distribution, $\Phi_e(E)$, in the volume of the studied material. In order to study the in-depth and volumetric AD distributions, it is possible to divide the volume of the material in subvolumes (voxels). In this way the energy fluence distribution in each one of these voxels can be obtained. Thus, the energy distribution of secondary particles can be computed as $\Phi_e(E) \times S$, being S the total section of the material (or voxel) surrounding the volume V.

It is known that the displacement of an atom occurs for particle energies higher than a certain cutoff energy E_c, corresponding to the threshold displacement energy of the target atom, T_d. On the other hand, all the simulation results are obtained normalized per incident photon or particle source. Thus, knowing the source fluence used in an specific study, it is possible to obtain the total number of AD, rewritten (4) after making some transformation:

$$N_{\mathrm{AD}} = N_a \Phi_0 S \int_{E_c}^{E_0} \sigma_d^*(E) \Phi_e(E)\, dE, \tag{5}$$

with

$$\sigma_d^*(E) = \frac{S}{V} \int_{E_c}^{E} \frac{\sigma_d(E')}{(-\mathrm{d}E'/\mathrm{d}x)}\, dE', \tag{6}$$

where the displacement cross section, $\sigma_d(E)$, is discussed in the next section.

A more common used way of expressing atom displacements is through the displacements per atom (dpa) magnitude, which can be obtained normalizing to the total number of atoms, N_{AD}/N_a. Furthermore, for compound materials all the constituent atomic species could be considered taking into account the relative fraction n_k of the k-atom in its crystalline sublattice. Thus the total displacements per atom can be calculated as the sum over all the atomic species: