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Computer simulation radiation damages in condensed matters

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Abstract. As part of the cascade-probability method were calculated the energy spectra of primary knocked-out atoms and the concentration of radiation-induced defects in a number of metals irradiated by electrons. As follows from the formulas, the number of Frenkel pairs at a given depth depends on three variables having certain physical meaning: firstly, C_d (E_0, h) is proportional to the average energy of the considered depth of the PKA (if it is higher, than the greater number of atoms it will displace); secondly is inversely proportional to the path length λ_1 for the formation of the PKA (if λ_1 is higher than is the smaller the probability of interaction) and thirdly is inversely proportional to E_d. In this case calculations are in satisfactory agreement with the experimental data (for example, copper and aluminum).

1. Introduction

In recent years in connection with the intensive development of nuclear power, studies of various physical processes in the near-Earth space, particularly in the Earth's radiation belts, the study of the influence of the electron, gamma and nucleon irradiations on the properties of materials has become one of the most important directions in solid state physics [1 – 5]. In the bombardment of solid bodies by charged particles, such as electrons, along the path of their movement are generated not only light particles such as secondary electrons (when energy is lost mostly by ionization of atoms), and atoms and ions of the medium which are the progenitor of the atom-atom cascades. The energy spectrum of primary knocked-out atoms (PKA) at various depths in the material depends on the energy, charge, mass of the incident particles and the type of target (atomic mass, density), integral and differential cross sections of particle-atom and atom-atom collisions and energy losses on ionization and excitation.

When propagating through medium the primary knocked-out atoms generate secondary knocked-out atoms, and then tertiary, etc. Ultimately, in the solid after the first process stage are formed the radiation defects such as vacancy-interstitial atom, divacancy and two knocked out atoms and so on [1, 2, 5 – 9].

2. The main results

Let us consider the multiple formation of PKA within the cascade-probabilistic method [10] and the possibility of using cascade-probability function in these processes. To define of the free path for the formation of the primary knocked out atoms (PKA) for electrons λ_1 we use the data of calculations of the cross sections σ_d (E_1). We remark that when calculating of the total free path R was taken into account the following. When decelerating of the electrons with initial energy E_0 there comes such

moment when their energy becomes less E_{th} (minimum energy for the formation of Frenkel pairs), and therefore further formation of PKA $P_1 (E_2)$ is not possible. Therefore, this "residue" was subtracted from the total free path. Let us compute the spectrum of PKA within the cascade-probabilistic method. We use a simple cascade-probability function [10].

Let the electron after going depth i-times have been elastically interacted with the formation of PKA. Their power spectrum $P_i (E_2)$ in the elementary act (normalized) can be written as:

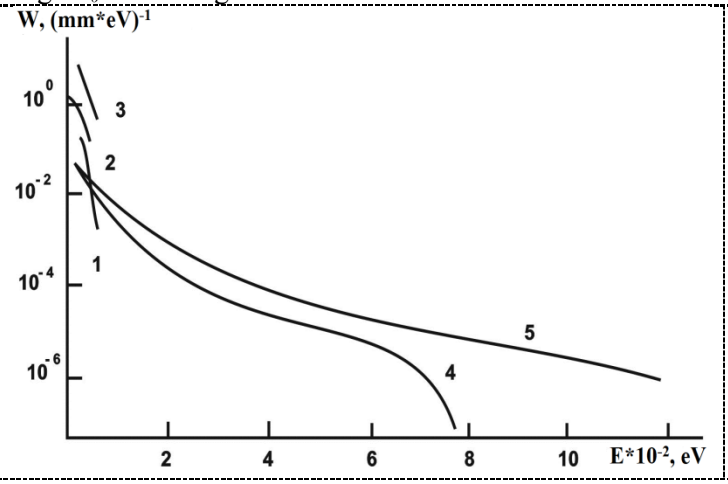
$$P_i(E_2) = \frac{d\sigma_i(E_1,E_2)}{dE_2\sigma_i(E_1)}, \quad \int_{E_d}^{E_{2max}^i} P_i(E_2)dE_2 = 1,$$

where $d\sigma/dE_2$ is the differential and $d\sigma_i(E)$ is the total cross section; E_1 is the energy of an electron at a depth h. As the second-knocked out atoms are taken into account by the cascade function ν (E_2) then the energy spectrum at a depth h for PKA can be too described by the function.

Here it is assumed that the electron and PKA retain the original direction of motion, the spectrum of PKA $W(E_0, E_2, h)$ at a depth h is determined by the formula:

$$W(E_0,E_2,h) = \sum_{i=0}^{\infty}\int_0^h \left(\frac{h'}{\lambda_1}\right)^i * \frac{1}{i!} e^{-\frac{h'}{\lambda_1}} P_i(E_2) e^{-\frac{h-h'}{\lambda_2}} (\lambda_2)^{-1} dh' \cdot (\lambda_1)^{-1}, \qquad (1)$$

where λ_2 is the free path of the atom-atom-atom displacements h′ is the depth of generating PKA. When electron irradiation with energy up to 10 MeV arise low energy PKA (their average energy is 200 eV) and therefore are not able to reach greater depths. Consequently, in (1) it is necessary to choose a real physical area of integration. It must obviously be of a size comparable to the mean free path of PKA. The energy of an electron at a depth h was defined as $E_1 = E_0 - \Delta E$, where ΔE is the ionization loss of electrons. These losses were calculated using a modified Bethe-Bloch formula. As a result of it was obtained that the value of *W (E0, E2, h),* depending on the E_2, is a decreasing function for all values of depths (Figure 1) and at low electron energies spectrum of PKA is much milder, at large E_0 is the tougher.



1 – 0,1 mm; 2 – 0,4; 3– 7; 4 – 4; 5 – 2

Figure 1. The spectra of PKA at different depths in the copper when it is irradiated with the electrons with the energy E_1 = 1 (1, 2) and 10 (3-5) MeV.

Let define the average energy $\overline{E_2}$ of PKA:

$$\overline{E_2} = \int_{E_d}^{E_{2max}} E_2 \frac{d\sigma}{dE_2} \cdot \left(\int_{E_d}^{E_{2max}} \frac{d\sigma}{dE_2}\right)^{-1}. \qquad (2)$$

From the calculations of the average energy of PKA it follows that it is slowly changing with the change of E_1 and does not exceed 200 eV (Figure 2).

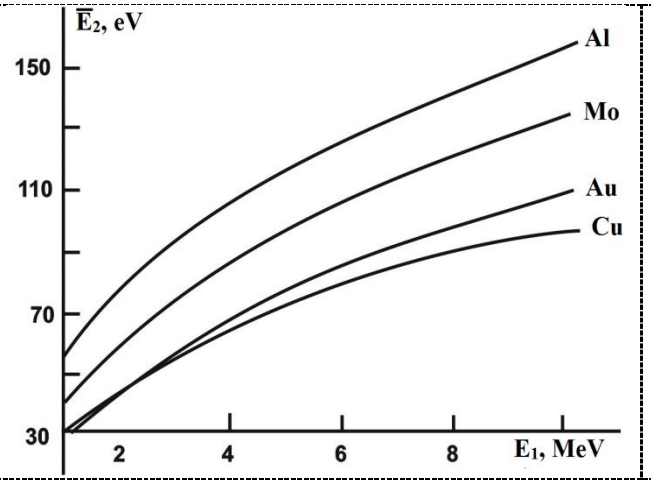


Figure 2. The dependence of the average transferred energy from energy of the electrons E_1 for different elements.

Further by means of the spectrum of PKA it can calculate the concentration distribution of Frenkel pairs in depth of the irradiated sample [10]:

$$C_d(E_0,h) = \int_{E_d}^{E_{2max}} \nu(E_2) W(E_0,E_2,h) dE_2, \tag{3}$$

where $\nu(E_2)$ is the cascade function; E_d is the threshold energy of displacement; E_{2max} is the maximum energy of the PKA.

As follows from the formulas (1), (3), the number of Frenkel pairs at a given depth depends on three variables having certain physical meaning: firstly, $C_d(E_0, h)$ is proportional to the average energy of the considered depth of the PKA (if it is higher, than the greater number of atoms it will displace); secondly is inversely proportional to the path length λ_1 for the formation of the PKA (if λ_1 is higher than is the smaller the probability of interaction) and thirdly is inversely proportional to E_d.

Let us calculate the relative concentration of Frenkel pairs N_d. The calculations will produce for thin foils, i.e. when the loss $\Delta E << E_0$, which corresponds to the initial part of $C_d(E_0, h)$. For the total number of displacements writes:

$$N_d = C_d(E_0,h)\Delta h \Phi t S,$$

where Δh is the thickness of the foil; S is the area the cross section of the sample; F is the flow; t is the time. Taking into account the total number of atoms in the sample for $N_d T = n_0 \Delta h S$ the relative concentration of point defects obtains [10]:

$$C_d(E_0,h) = 0{,}4\Phi t \overline{E_2}(h) \cdot (n_0 \lambda_1(E_0) E_d)^{-1}. \tag{4}$$

To define energy dependence of the total number of displacements per one incident electron, let us integrate (3) in depth from 0 to h_d (the maximum depth on which the electron forms another PKA), i.e.

$$C_d(E_0) = \int_0^{h_d(E_0)} C_d(E_0,h) dh. \tag{5}$$

Let us compare our calculations with the experimental values on a gain of residual electrical resistivity $\Delta\rho$ at low temperatures [2] (T ≃ 20, 4 K). In this case $\Delta\rho$ was determined by the formula:

$$\frac{\Delta\rho}{\Phi t} = \Delta\rho_f C_d(E_0) \cdot (n_0 h d(E_0))^{-1} \cdot 100\%, \tag{6}$$

where $\Delta\rho_f$ is the increase in the electrical resistivity of Frenkel pairs.

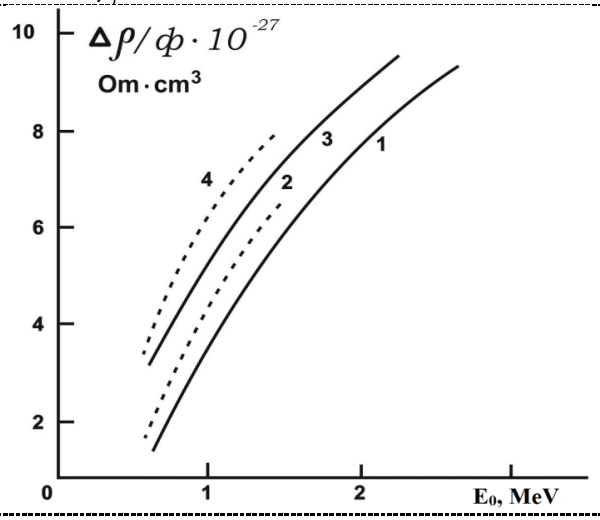


Figure 3. Dependence of the growth of the residual electrical resistivity in the Cu (1) and Al (3) on the energy of electrons: 1, 3 – calculation; 2, 4 – Experiment [2].

When calculatings of $\Delta\rho/\Phi t$ were used the following values for Al and Cu: $\Delta\rho_{Al}$ = 3, $4\cdot10^{-6}$ ohm·cm/at. %, $\Delta\rho_{Cu}$ = 1, $3\cdot10^{-6}$ ohm·cm/at. %. The dependences $\Delta\rho(E_0)/\Phi t$ are shown in Figure 2. In the interval of electron energies E_0 = 0.6 – 1.3 MeV (corresponding to the experiment [2]) calculated curves differ from the experimental no more than 20%.

3. Conclusion

1. With the use of the simple cascade-probability function an analytical expression for the energy spectrum of primary knocked-out atoms (PKA) and the concentration of radiation-induced defects have been received. The calculations of these functions for copper and aluminum were produced.
2. The calculation of the dependence of the electrical resistance on the energy of the electrons gives satisfactory agreement with experiment.

Acknowledgments

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