

Dynamic model of the threshold displacement energy

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Abstract. A dynamic (cascade-probability) model for calculating the threshold displacement energy of knocked-out atoms (E_d) was proposed taking into account the influence of the instability zone (spontaneous recombination). General expression was recorded for E_d depending on the formation energy of interstitial atoms E_f and vacancies E_i , on the energy transfer coefficient α and the number of interactions i needed to move the atom out of the instability zone. The parameters of primary particles were calculated. Comparison of calculations with experimental data gives a satisfactory agreement.

1. Introduction

As it is known, the interaction of the neutral and charged particles (electrons, ions, gamma rays, neutrons, etc.) with materials forms the radiative defects of vacancy and interstitial types of various sizes and configurations [1 – 4]. This significantly changes the structure and properties of the substance [5 – 10].

For calculation of the concentration of radiative defects in the materials the minimum energy required for the formation of a displaced atom (from the node-crystalline lattice), or so-called primary knocked-out atom (PKA) should be known. In radiation physics, this energy is called the threshold displacement energy and expressed as E_d or T_d . The value of E_d was qualitatively assessed for the first time by Seitz based on the following considerations. The energy needed for separation of the atom or ion (the sublimation energy) from the solid surface in common solid crystal $E_c \sim 5$ eV. Sublimation (evaporation) takes place on the surface of the crystal, where it is enough for separation to overcome only the half of interatomic bonds compared with an atom located inside the crystal. The binding energy of the inner atom therefore is approximately equal to 10 eV. If the atom moves slowly from the lattice node along the path of least resistance to some interstitial position, thereby allowing the neighboring atoms to return to the original position or if there is an adiabatic motion, this process requires energy, which is approximately equal to $2E_c$. In fact, knocked-out atom receives a sharp blow and enters the interstitial position almost unable to return. Generally, the atom moves not along the line of least resistance, and the neighboring atoms do not have time to relax. A reasonable estimation for the value of consumed energy (according to [1, 2]) is $\sim 4 - 5 E_c$, i.e. 20 – 25 eV, and, therefore, E_d is equal to 25 eV. It should be noted that this estimation is quite crude, since it does not account the real picture of the formation of interstitial atoms and vacancies (Frenkel couples). It is clear that such non-adiabatic formation of the displaced atom must depend both on the PKA energy E_2 and the material type and the direction of particles emission. The higher the PKA energy, the faster it moves, and the better such motions are. At the same time, the movement time should be much less than the atoms relaxation time. If these times are comparable, the interstitial atom formation process is close to adia-



batic and the liminal formation energy must be less than the above mentioned $4E_c$ and is close to the E_c . This leads to the fact that we have a distribution on the threshold energy, i.e. in the energy range of $0 \sim 200$ eV the formation of stable Frenkel couple (vacancy + interstitial atom) is less than one.

We have proposed a dynamic (cascade-probability) model of calculation of the threshold displacement energy.

2. Fundamentals of the model

The average energy of the atom displacement can be obtained from the athermal approach more strictly than in [1, 2]. Since the instability zone (spontaneous recombination) exists around the vacancy [3], kicked-out atom is necessary to undergo several collision (i) to get beyond it. In this case, basically, the atom will lose energy by elastic collisions with surrounding atoms. In the approximation of solid bodies, energy spectrum $\omega(E_2)$ of the secondly kicked-out atoms (from PKA) is described by uniform distribution ($\omega(E_2)dE_2 = AdE_2$). Moreover, the energy transfer coefficient α (i.e., the fraction of energy transmitted by primary atom to secondary) can be determined by the average energy of kicked-out atoms:

$$\overline{E_2} = \frac{\int_0^{E_{2\max}} E_2 \omega(E_2) dE_2}{\int_0^{E_{2\max}} \omega(E_2) dE_2} = \frac{E_{2\max}}{2}. \quad (1)$$

Here the good approximation gives $\alpha = 0.5$.

The average collisions number \bar{i} can be determined using cascade-probability function $\psi_i(h)$:

$$\bar{i} = \sum i \cdot \psi_i(h), \quad (2)$$

where [11]

$$\psi_i(h) = \frac{1}{i!} \left(\frac{h}{\lambda} \right)^i \exp\left(-\frac{h}{\lambda}\right).$$

Here h is the depth of observation, λ is interaction path, $\lambda = 1/\sigma n$, σ is total cross section, n – the number of atoms per cubic centimeter.

Since

$$\sum_{i=0}^{\infty} \psi_i(h) = 1, \quad \bar{i} = h/\lambda. \quad (3)$$

x , y , z and r coordinates may be considered instead of h :

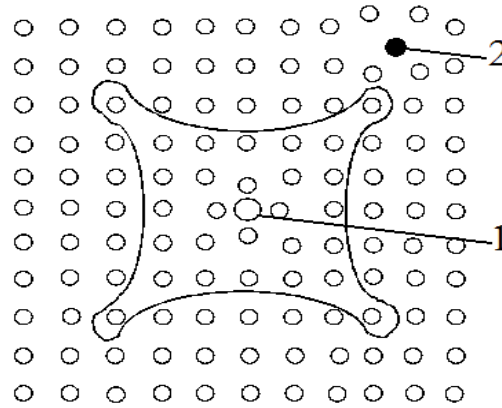
It follows that the i value depends on the motion direction of the atom in the instability zone. Typical view of such zone is shown in Figure 1.

In general

$$\bar{i} = \frac{1}{N} \sum_1^N i(x, y, z). \quad (4)$$

Where N is the number of points, $i(x, y, z)$ is the i values in x , y , z points on the outer surface of spontaneous recombination zone. Ultimately, the value of E_d is determined as follows:

$$E_d = \frac{E_v + E_f}{(1 - \alpha)^i}. \quad (5)$$



1 – vacancy; 2 – interstitial atom

Figure 1. The instability zone for knocked-out atom (flat picture).

3. Results and discussion

Regarding (1)-(5) and $E_f + E_v = 5$ eV and $\alpha = 0.5$ the values of i and E_d are to be calculated. The results are given in Table 1. It can be seen that the experimental data are in agree with calculations

Table 1. Threshold energy of the atoms and the incoming particles, and the average number of interactions.

Threshold energy	Al	Ti	Cu	Mo	Ag	Au
$E_d',$ (eV) [12], experiment	32	29	22	37	28	35
$E_d,$ (eV, calculated)	30.3	28.3	2.4	37.3	26.4	32.5
E_{th}^e of the electron, (MeV)	0.3	0.44	0.44	0.87	0.78	1.365
E_{th}^p of the proton, (eV)	231	360	360	900	760	1730
E_{th}^α of the α -particle, (eV)	71	100	100	240	200	450
\bar{i}	2.6	2.5	2.1	2.9	2.4	2.7

Thus, in our view, it is possible to introduce the following definition: "The threshold displacement energy E_d is the minimum energy that should be given to an atom of the material so that it is displaced from the lattice site and get out of the instability zone after i interactions, forming a stable Frenkel pair".

Radiation physics is characterized by the existence of the minimum energy of damaging particles, in which the defect formation is possible. In this regard, let's consider the elementary act of interaction of primary particles with atoms, leading to the formation of PKA.

For the test process, the threshold kinetic energy E_{th} of the incoming particles has been calculated. Let's consider the process of elastic collision of particles possessing kinetic energy E_1 , with fixed atom. If the primary particle is unrelativistic and heavy, the maximum kinetic energy E_{th}^i , that it should have for knocking out an atom is equal to:

$$E_{th}^i = (m_1 + m_2)^2 / 4m_1 \cdot m_2 \cdot E_d. \quad (6)$$

Where m_1 and m_2 are the mass of the incoming particle (e.g. ion) and fixed atom, respectively. Or effective separation of an atom from the crystal lattice the inequality should be saved: $E_{2\max} \geq E_d$ [3, 11].

During the electron-atom collisions $m_1 \ll m_2$. For example, for $E_d = 20$ eV [5], $E_1 \geq 0.1$ MeV, which indicates the inapplicability of the non-relativistic mechanics for electrons [12]. Consequently, for the electron irradiation in the problems related to the formation of displaced atoms, relativistic kinematics should be used so the maximal value of E_{th}^e , which should have a primary particle-conductive identified the following equation:

$$E_{th}^e = \frac{\sqrt{4m_1^2 c^4 + 2E_d \cdot m_2 c^2} - 2m_1 c^2}{2}. \quad (7)$$

Table 2 shows the results of E_{th} calculations for different elements in electron, proton and alpha radiation. As the table shows, with increasing atomic number the value of E_{th} is generally increased.

However, there are deviations from this relationship, for example, molybdenum, which is associated with the difference in the threshold displacement energy for this item

4. Conclusions

1. With the use of cascade-probability method the dynamic (cascade-probability) model developed for calculating the threshold displacement energy of atoms a stable Frenkel couples.
2. The energy of transfer rate, the number of interactions, the threshold displacement energy E_d and the maximum energy for electrons, protons, alpha particles, reaching the used in defects in aluminum, titanium, copper, molybdenum, silver and gold was calculated. The available experimental data are satisfactorily described the proposed model.

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