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Abstract

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ON THE IONIZATION MECHANISM OF THE FORMATION OF STRUCTURAL DISTURBANCES IN CRYSTALS

In a number of experimental works ([1,2]) it has been shown that the efficiency of destruction of the crystal lattice increases when the energy of the penetrating radiation is lowered, although the cross section for elastic displacements, as a rule, decreases in this case. Moreover, in individual cases ([3]) the formation of defects in crystals is observed at energies of the acting radiation considerably below the threshold. These facts have led to the assumption that radiation structural defects may be formed as a result of excitation and ionization of electrons ([4,5]). Ionization mechanisms of defect formation are of primary importance for nonconducting crystals, since the relaxation time of a nonequilibrium charge distribution is determined by the quantity

$$\tau_0 = \varepsilon/\sigma_0,$$

where ε is the dielectric permittivity, and σ_0 is the conductivity of the crystal; for metals this quantity is too small.

We shall show, using as an example the interaction of slow electrons (10^4–10^5 eV) with the lattice of a valence crystal, that the processes of ionization of atomic electron shells can play a considerably greater role in defect formation than is usually assigned to them.

The probability that a lattice atom will leave its site for an interstice is proportional to the ratio of the time interval during which the atom has sufficient energy to overcome the potential barrier to the period of oscillations:

$$W \simeq \frac{\tau}{T}. \tag{1}$$

For a crystal in equilibrium $W = \exp(-U/kT)$, where U is the height of the potential barrier.

When ionizing radiation acts on a crystal, a lattice atom, as a result of multiple ionization, may also for some time τ find itself above the potential barrier and,

consequently, with a certain probability, pass into an interstice. When slow electrons pass through a crystal, lattice atoms can with high probability enter a state of multiple ionization as a result of the ejection of a K-shell electron and subsequent Auger transitions ([6,7]). Thus, the cross section for multiple ionization may be written as the cross section for K-ionization multiplied by the product of the probabilities of successive Auger transitions,

$$\sigma = \sigma_K \prod_i (1 - \eta_i), \tag{2}$$

where η_i is the fluorescence yield for the corresponding x-ray series.

The potential well in which a lattice atom is located in a crystal is created by the superposition of various forces of interatomic interaction: Coulomb, exchange, van der Waals, etc.

The binding forces in a valence crystal are determined mainly by the Coulomb repulsion of atomic cores and the exchange interaction of valence electrons. Assuming that multiple ionization extends only to the shells of atomic cores, one can express the change in the potential–

of the energy of a multiply ionized atom in the following way:

$$\Delta V = \sum_k \sum_j \frac{(Z_i^* - \sigma_i)(Z_j - \sigma_j)e^2}{r_{ij}^k} - \sum_k \sum_j \frac{(Z_i - \sigma_i)(Z_j - \sigma_j)e^2}{r_{ij}^k} - (Z_i^* - Z_i)e \int_{r_0}^{\infty} \left(1 - \frac{1}{\varepsilon}\right) \frac{e}{r^2}\, dr. \tag{3}$$

Here $Z_i = Z_j$ is the charge of the atomic cores in the crystal; $\sigma_{i,j}$ is the screening constant due to valence electrons; r_{ij}^k is the distance from the i-th atom under consideration to all j atoms of the k-th coordination sphere; ε is the dielectric permittivity; r_0 is the radius of the sphere inside which the additional charge causing polarization of the medium is located; Z_i^* is the charge of the multiply ionized atomic core.

The change in potential energy in the case considered may greatly exceed the magnitude of the potential barrier, reaching values of more than 10 eV. This situation is shown schematically in Fig. 1. Upon emission of Auger electrons the atom is given recoil energy, which is expressed by the quantity

$$E_0 = \frac{m}{M} E_k, \tag{4}$$

where m is the electron mass, M is the atomic mass, and E_k is the kinetic energy of the Auger electron. E_0 may reach several electron volts. Thus an atom passing into a state of multiple ionization is simultaneously given an impulse, owing to which it may leave its lattice site by more than one interatomic distance.

Fig. 1

Figure 1: Fig. 1

Fig. 1

The cross section of the displacement process described can be written in the form:

$$\Sigma_0 \simeq \sigma_K \prod_i (1-\eta_i)\frac{\tau_i}{T}. \tag{5}$$

In this case τ_i is the lifetime of the multiply ionized state. Estimates show that $\Sigma_0 \simeq 10^{-25}$–10^{-27} cm^2. The Varley mechanism (5), realized in ionic crystals, may be regarded as a particular case of the mechanism described.

The formation of radiation defects, in accordance with the mechanism described, should be sufficiently effective in the region of threshold and subthreshold energies for elastic displacements. This may, to a certain extent, explain the observed ambiguity in the determination by various authors ([8],[9]) of the threshold energies for the formation of radiation defects.

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Note: Figure translations are in progress. See original paper for figures.