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Energy criterion for the stability of defects in semiconductor crystals to the action of external fields

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Abstract. A criterion for the stability of defects in semiconductor structures to the action of magnetic and electric fields, electromagnetic radiation, acoustic waves, mechanical stresses has been formulated. Analytical relations have been obtained for the threshold parameters of external fields, at which transformation of defects was observed. The results of calculations of the threshold values for the magnetic field induction that cause a change in the state of dislocations and defect clusters in semiconductor crystals have been presented.

Keywords: semiconductor, defect, magnetic field, electromagnetic field, acoustic wave, mechanical stress.

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1. Introduction

The study of the stability of defects to the action of weak external fields, in particular, magnetic, electric and electromagnetic ones, acoustic (sound) waves, mechanical stresses is of interest from the viewpoint of both predicting stability of the characteristics of semiconductor crystals in time and controlling their structure. Thus, the effects of transformation of dislocations and point defects in semiconductor and dielectric crystals, stimulated by the nonthermal action of microwave electromagnetic radiation, as well as by weak magnetic fields, are, on the one hand, paradoxical, and, on the other hand, are reliably confirmed experimentally [1–6]. The nontriviality of the situation lies in the fact that the values of parameters of external fields, namely: radiation frequency, magnetic field induction and electric field strength, satisfy the conditions:

1. The quantum of energy of electromagnetic radiation is much less not only than the activation energy of elementary act for changing the state of defect, but also than the average energy of thermal fluctuations: $\hbar\omega_{em} << kT$ (ω_{em} is the angular frequency of the electromagnetic wave, $\hbar$ – Planck constant, k – Boltzmann constant, T – absolute temperature), and the intensity of radiation or duration of its exposure are such that they do not cause heating the material.

2. The energy transferred to a paramagnetic particle in a uniform magnetic field with the induction B is such that $\mu_B B << kT$ (μ_B is Bohr magneton).

3. The energy of a charged particle (ion) in a uniform electric field with the strength E is limited by the inequality: $eEd << kT$ (e is the electron charge, d – distance between two minima of potential energy in the crystal lattice). It is assumed that the electrical conductivity of the material can be neglected, which occurs in dielectrics or space charge regions near the surface of semiconductors depleted of major charge carriers.

Thus, the question arises as to why such small influences are not lost against the background of thermal disturbances in crystal structures with a characteristic scale kT. To substantiate the physical nature of these extraordinary phenomena, the concept of both resonance vibrations of electrically charged edge dislocations and clusters consisting of pairs of cation-anion defects (donor-acceptor complexes) [6] and the occurrence of spin-dependent reactions, *i.e.*, singlet-triplet transitions in radical pairs of defects [1–3, 6].

At the same time, it should be specially noted that the above criteria for the smallness of the parameters of external influences are valid only for point defects. However, both dislocations and defect clusters are extended objects with a rather significant microscopic volume. Then the question arises as to the ratio of the energy of the external field, localized in their volume, to the thermal energy kT. This approach (let us call it energetic) will make it possible to estimate the threshold values of the parameters of external fields at which defects acquire the ability to change their state.

This work is aimed at consideration of the energy criterion for the stability of defects to the action of external fields.

2. Analysis of the loss of stability by defects under the action of external fields on semiconductor structures

Loss of stability is understood as transformation of defects, *i.e.*, a change in their state when external fields are applied to a semiconductor crystal. In its turn, transformation is understood as a sequence of elementary acts of detachment and subsequent displacement of dislocations, decay of donor-acceptor pairs that form defect clusters as well as further diffusion of ions [6].

Transformation of defects is a thermally activated process with an activation energy E_a [7]. Therefore, elementary acts of transformation of defects are random events that are characterized by a random variable – the time before fluctuation of energy $E_f = E_a$ of particles (ions, atoms), of which the defect consists [7]. For example, the displacement of dislocations is caused by a sequence of random events – elementary thermally activated acts of detachment from stoppers, formation of double bends. The decay of a cluster of defects is based on a sequence of thermally activated acts of dissociation of individual donor-acceptor pairs and ion diffusion.

The time before the fluctuation energy of particle with the value E_a obeys the distribution with the function $F(t)$ [7]:

$$F(t) = 1 - \exp\left[-\left(\frac{t}{\tau_f}\right)\right], \qquad (1)$$

where τ_f is the average time between two successive fluctuations of the value $E_a = E_f$ of particle, that is equal to:

$$\tau_f = \tau_0 \exp\left(\frac{E_a}{kT}\right), \qquad (2)$$

where τ_0 is the pre-exponential factor that coincides by its order of magnitude with the period of thermal vibrations of particle in the semiconductor lattice.

Consequently, the elementary act of transformation of a defect requires initiating thermal energy, causing energy fluctuation $E_f = E_a$ of at least one particle of which it consists. Thus, the energy criterion for the stability of defects in semiconductor crystals to the action of external fields is as follows: for a defect to perform an elementary act of transformation during the action of an external field, it is necessary that the energy of this field, localized in the bulk of the defect, was equivalent to kT_{1f}, and T_{1f} being understood as the temperature of the semiconductor structure at which during the time t of external field action on a defect with its volume V, at least one particle will experience energy fluctuations with their value E_a.

From the mathematical viewpoint, the energy criterion for the stability of defects to the action of external fields is written in the form:

$$\int w dV = kT_{1f}, \qquad (3)$$

where w is the bulk energy density of the external field (in a general case, it is a function of coordinates), dV – element of the defect volume V.

In the case when the bulk density of the field energy w is not a function of coordinates (homogeneous magnetic and electric fields, plane harmonic electromagnetic and acoustic waves), we obtain that the threshold (minimum) value w_{th}, at which the loss of stability of a defect with the volume V takes place, is equal to:

$$w_{th} = \frac{kT_{1f}}{V}. \qquad (4)$$

To determine the temperature, at which, during external field action, at least one particle of the defect will experience energy fluctuations of the value E_a, the following equation can be used:

$$VNF(t) = 1, \qquad (5)$$

where N is the number of atoms per unit volume of semiconductor, and VN is the number of particles in the defect.

Taking into account (1), we represent the relation (5) as follows:

$$1 - \exp\left[-\left(\frac{t}{\tau_{1f}}\right)\right] = \frac{1}{VN}, \qquad (6)$$

moreover, τ_{1f} is such an average time between two successive fluctuations, at which during the time t of the action of an external field in a defect with a number of particles VN, one of them experiences energy fluctuation of the value E_a:

$$\tau_{1f} = \tau_0 \exp\left(\frac{E_a}{kT_{1f}}\right). \qquad (7)$$

Assuming that the number of particles in the defect is $VN >> 1$, then the right-hand side of (6) tends to zero, and therefore, during the entire time of the external field action, the exponent tends to unity. The latter means that $t << \tau_{1f}$. Thus, this exponent can be expanded in a series and limited to its first term by t/τ_{1f}:

$$\exp\left[-\left(\frac{t}{\tau_{1f}}\right)\right] = 1 - \frac{t}{\tau_{1f}}. \qquad (8)$$

Summing up (6) to (8), we have:

$$\frac{t}{\tau_0 \exp\left(\dfrac{E_a}{kT_{1f}}\right)} = \frac{1}{VN}. \qquad (9)$$

It follows from (9) that

$$T_{1f} = \frac{E_a}{k \ln \dfrac{VNt}{\tau_0}}. \qquad (10)$$

Taking into account (4) and (10), for the stability criterion we have the following expression:

$$w_{th} = \frac{E_a}{V \ln\left(\frac{VNt}{\tau_0}\right)}. \tag{11}$$

Thus, the threshold value of the bulk energy density of the external field is proportional to the activation energy of elementary acts of defect transformation. For the same duration of the applied external fields, the higher the threshold value of the bulk density of the field energy, the lower the volume of defect. Consequently, if the value of the bulk energy density of the external field acting on the crystal is such that defects with the volume V_1 lose their stability, then defects with any other volume greater than V_1 change their state. For a defect of a given volume, the greater the threshold value of the bulk energy density of the external field, the shorter the duration of the action of the latter.

From the physical viewpoint, the mechanism of action of these fields on crystal defects is as follows. A homogeneous electric field and electric component of a plane harmonic electromagnetic wave interact with electrically charged particles of edge dislocations, as well as defect clusters. A homogeneous magnetic field and magnetic component of the electromagnetic wave interact with the magnetic moments of particles that form the defects. Plane harmonic sound wave and mechanical stresses deform chemical bonds.

The bulk energy densities of homogeneous magnetic and electric fields w_B and w_E are, respectively, equal to [8]:

$$w_B = \frac{B^2}{2\mu\mu_0}, \tag{12}$$

$$w_E = \frac{\varepsilon\varepsilon_0 E^2}{2}, \tag{13}$$

where μ is the magnetic permeability of semiconductor, ε – dielectric constant of the crystal; μ_0 – magnetic constant, ε_0 – electrical constant.

The relation for the bulk density of the elastic strain energy w_{M1} under tension (compression) has the form [9]:

$$w_{M1} = \frac{\sigma^2}{2E_Y}, \tag{14}$$

where σ is the tension (compression) stress, E_Y – Young's modulus of a semiconductor crystal.

The bulk density of the potential energy of elastic deformation w_{M2} during shear is represented by the expression [9]:

$$w_{M2} = \frac{\tau^2}{2G}, \tag{15}$$

where τ is the shear stress, and G – shear modulus of the semiconductor.

With regard to the electromagnetic field of the microwave range, we will use the average value of the bulk energy density. This is caused by the fact that, as a rule, the duration of the application of the field to the semiconductor structure is much longer than the period of oscillations of the electromagnetic wave. Therefore, it is advisable to carry out averaging of the bulk energy density over the time of action of an electromagnetic field on the crystal. The average value of the bulk energy density of the electromagnetic field $\overline{w_{em}}$ for a plane electromagnetic wave propagating in a homogeneous medium without electrical conductivity takes the form [8]:

$$\overline{w_{em}} = \frac{\varepsilon\varepsilon_0 E_m^2}{2} = \frac{B_m^2}{2\mu\mu_0}, \tag{16}$$

where E_m and B_m are the amplitude values of the electric and magnetic components of the electromagnetic wave, respectively.

The time-averaged bulk energy density $\overline{w_S}$ of a harmonic plane traveling acoustic wave is [9]:

$$\overline{w_S} = \frac{p_m^2}{2\rho\upsilon_S^2}, \tag{17}$$

where $p_m = \rho\upsilon_S\upsilon_m$ is the maximum sound pressure (pressure amplitude), ρ – density of the material, υ_S – sound speed, υ_m – maximum vibrational velocity of particles (amplitude of the vibrational velocity).

Substituting (12)–(17) into (11), we obtain the following relations for the threshold values of the parameters of external fields at which the loss of stability of defects in semiconductor structures is observed:

$$B_{th} = \left[\frac{2\mu\mu_0 E_a}{V \ln\left(\frac{VNt}{\tau_0}\right)}\right]^{1/2}, \tag{18}$$

$$E_{th} = \left[\frac{2E_a}{\varepsilon\varepsilon_0 V \ln\left(\frac{VNt}{\tau_0}\right)}\right]^{1/2}, \tag{19}$$

$$B_{mth} = \left[\frac{2\mu\mu_0 E_a}{V \ln\left(\frac{VNt}{\tau_0}\right)}\right]^{1/2}, \tag{20}$$

$$E_{mth} = \left[\frac{2E_a}{\varepsilon\varepsilon_0 V \ln\left(\frac{VNt}{\tau_0}\right)}\right]^{1/2}, \tag{21}$$

$$\sigma_{th} = \left[\frac{2E_Y E_a}{V \ln\left(\frac{VNt}{\tau_0}\right)} \right]^{1/2}, \tag{22}$$

$$\tau_{th} = \left[\frac{2GE_a}{V \ln\left(\frac{VNt}{\tau_0}\right)} \right]^{1/2}, \tag{23}$$

$$p_{mth} = \left[\frac{2\rho\upsilon_S^2 E_a}{V \ln\left(\frac{VNt}{\tau_0}\right)} \right]^{1/2}. \tag{24}$$

Note that $B_{th} = B_{mth}$ and $E_{th} = E_{mth}$.

The above formulas indicate the volume of the defect V. By the volume of an edge dislocation V_d, we mean the product of the area of its core $S_d = \pi r_d^2$ by the length L_d, that is:

$$V_d = \pi r_d^2 L_d, \tag{25}$$

where r_d is the radius of the dislocation core (is of the order of several lattice constants).

The volume of a cluster of defects V_c in the particular case of its spherical shape is equal to:

$$V_c = \frac{4}{3}\pi r_c^3, \tag{26}$$

where r_c is the radius of the cluster.

Thus, the threshold values of the parameters of external fields are proportional to the square root of the activation energy of elementary acts of defect transformation. With the same duration of the applied external fields, each defect can be assigned to a certain threshold value of the parameter of the field causing its transformation. The higher the latter field, the smaller the volume of the defect, *i.e.*, the smaller the length and radius of the dislocation core, the radius of the defect cluster. For a defect of a given volume, the higher the threshold value of the parameter, the shorter the duration of action of the external field on semiconductor.

The energy stability criterion analyzed in this work predicts a number of important features of the effect of external fields on the defect subsystem of semiconductor structures:

1. Presence of threshold values of parameters of the fields that cause transformation of defects.

2. Saturation effects in changes in the characteristics of crystals that are sensitive to an external field, since with an increase in the values of the field parameters, the maximum possible number of defects change their state.

3. The quadratic dependence of the observed effects on the parameters of external fields, in view of a similar functional dependence of the volume density of the field energy, and, consequently, the field energy localized in the volume of the defect.

These features were experimentally observed in changes in magnetically sensitive quantities, in particular, the paths of dislocations in semiconductor and dielectric crystals under action of magnetic fields on them [1, 2, 10].

3. Calculation of threshold values of magnetic field induction

Let us estimate the threshold values B_{th} for dislocations and defect clusters in GaAs crystals exposed to magnetic fields of duration $t = 60$ s. Let the length of the edge dislocation $L_d = 10^{-6}$ m, and the radius of its core is equal to two lattice constants, which is $5.65325 \cdot 10^{-10}$ m in gallium arsenide [11]. Taking into account the value $N = 4.42 \cdot 10^{28}$ m^{-3} for gallium arsenide [11] and assuming that $\mu = 1$, $\tau_0 = 1.25 \cdot 10^{-13}$ s, $E_a = 1$ eV, as a result of calculation by using the formulas (18) and (25), we get $B_{th} = 4.7 \cdot 10^{-2}$ T. For a cluster of spherical shape defects with $r_c = 10^{-8}$ m, in accordance with (18) and (26), we have $B_{th} = 4.6 \cdot 10^{-2}$ T. The results obtained agree with the values of magnetic field induction in the works of the authors on studying the long-time non-monotonic changes in the intensity of the photoluminescence bands of GaAs semiconductor compounds stimulated by this field [6].

4. Conclusions

Loss of stability, *i.e.*, a change in the state of defects in semiconductor structures occurs when localizing in their volume the external field energy equivalent to thermal energy, at which, during field action, at least one particle, of which the defect consists, will experience fluctuation of energy with the value equal to that of activation energy of an elementary act for defect transformation. Each defect is characterized by a certain threshold (minimum) value of parameter of the external field that causes a change in its state. Threshold values of induction and strength of magnetic, electric and electromagnetic fields, mechanical stresses, sound pressure are proportional to the square root of the activation energy. For the same duration of the applied external fields, the larger these threshold values, the smaller the volume of the defect. For a defect of a given volume, the higher the threshold value of the external field parameter, the lower the duration of its action. The results of calculations of the threshold values of the magnetic field induction for dislocations and defect clusters in semiconductors have been presented. The obtained values are agreed with those used by the authors when studying the effect of magnetic fields on the change in the intensity of the photoluminescence bands of semiconductor crystals. The energy stability criterion, in particular, explains the following effects experi-mentally observed under the influence of magnetic fields: threshold character, quadratic dependence, saturation in changes in magnetically sensitive quantities of semi-conductors with increasing induction. The analyzed energy approach, together with the concept of resonance phenomena and spin reactions enable to form a more complete picture to understand transformation of crystal defects under the action of external fields.

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Енергетичний критерій стійкості дефектів у напівпровідникових кристалах до дії зовнішніх полів

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Анотація. Сформульовано критерій стійкості дефектів у напівпровідникових структурах до дії магнітних та електричних полів, електромагнітного випромінювання, акустичних хвиль, механічних напружень. Отримано аналітичні співвідношення для порогових параметрів зовнішніх полів, у яких спостерігається трансформація дефектів. Наведено результати розрахунків порогових значень індукції магнітного поля, що викликають зміну стану дислокацій та кластерів дефектів у напівпровідникових кристалах.

Ключові слова: напівпровідник, дефект, магнітне поле, електромагнітне випромінювання, акустична хвиля, механічне напруження.