Semiconductor Physics, Quantum Electronics & Optoelectronics, 2025. V. 28, No 3. P. 267-276.

Semiconductor physics

Physical-statistical principles of analysis of defect transformations in semiconductor structures under influence of magnetic and electromagnetic fields

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Abstract. The paper presents a methodology of the physical-statistical analysis of defect transformations in semiconductor structures under action of magnetic and electromagnetic fields. The probability-energy criterion of defect stability to external fields is analyzed. The mathematical foundations of the physical and statistical analysis of reconstruction of the defect structure of semiconductors under action of magnetic and electromagnetic fields are formulated. A probabilistic-physical study of time transformations of radiative recombination spectra due to action of microwave radiation and magnetic-field treatments is carried out. The mechanisms of defect reorganization under action of magnetic and electromagnetic fields on semiconductor structures are considered.

Keywords: point defect, dislocation, defect cluster, magnetic field, microwave radiation.

https://doi.org/10.15407/spqeo28.03.267
PACS 05.40.-a, 41.20.-q, 71.55.Eq

Manuscript received 10.06.25; revised version received 07.07.25; accepted for publication 03.09.25; published online 24.09.25.

1. Introduction

A large number of works are devoted to the effects of transformation of dislocations and point defects in semiconductors, stimulated by non-thermal action of ultra-high-frequency electromagnetic radiation [1–16] and weak magnetic fields [17–23]. The peculiarity of the experiments is that the parameters of the external fields, namely the electromagnetic radiation frequency and magnetic field induction, correspond to the energy of an electromagnetic radiation quantum or a paramagnetic particle much smaller not only than the defect activation energy but also than kT (the product of the Boltzmann constant and the absolute temperature).

Therefore, the following important questions arise: Why are such small effects not lost on the background of thermal disturbances in crystalline structures and lead to defect reorganization? What is the smallness criterion for the characteristics of these effects and what are the threshold (minimum) values of the external field parameters at which the defects become able to change their state? On the other hand, external effects with different deterministic values of force field indicators were used in numerous experiments. At the same time, the patterns of the defect transformations showed a similar picture. Hence, the question arises: Why does this happen?

It may be assumed that the specificity of the observed phenomena is based on the fact that they have both a physical and a stochastic nature. Therefore, to answer all the questions outlined in this paper, a physical-statistical approach to a study of the influence of external actions (magnetic field and microwave radiation) on transformation of the defect subsystem in semiconductors is presented, taking into account both these natures.

It should be also noted that traditionally, microwave processing is accompanied by thermal heating of an irradiated material [16, 24–37], and that the idea of non-thermal action is characteristic not only of semiconductors, but also of liquids and biological systems [38–43]. In this paper, we will not consider the latter systems, but concentrate on non-thermal microwave irradiation and pulsed magnetic field processing of semiconductors.

2. General principles of the physical-statistical method for studying transformations of the defect subsystem of semiconductors under influence of external fields

The probabilistic-physical (other names: physical-statistical, deterministic-stochastic) approach to a study of the influence of external actions (magnetic field and microwave radiation) on transformations of the defect subsystem of semiconductors takes into account that the evolution of this system and its mechanisms are subject not only to dynamic laws, but also to the laws of statistics.

The components of the physical-statistical method for studying transformations of defects in semiconductor structures stimulated by action of magnetic and electromagnetic fields are as follows:

1. Probabilistic-energetic concept of defect stability to the action of external fields.
2. Physical-statistical modeling of the laws of evolution of the defect subsystem of semiconductor structures under the influence of a magnetic field and microwave radiation.
3. Deterministic-stochastic nature of the mechanisms of defect reorganization under the action of external fields.

3. Probability-energetic criterion of defect stability in semiconductor structures to action of magnetic and electromagnetic fields

To understand the reason for the loss of stability by defects, which is manifested by a change in their state under action of external fields on a semiconductor, it is necessary to take into account the fact that both dislocations and defect clusters are extended objects. They consist of a large number of particles and are characterized by a certain volume. Each of the defect particles experiences fluctuations in energy of a thermal origin. These thermal fluctuations under certain conditions cause jumps of the particles between the minima of symmetric double potential wells, which change both their state and the reconstruction of the defect as a whole.

It is quite logical to compare the values of the energy of an external field localized in the bulk of a defect and the energy scale of thermal fluctuations of the defect constituent particles. Such a phenomenological approach, called energetic approach, allows us to estimate potential stability of the defect to the action of the external fields without considering internal mechanisms stimulating its transformation. Since fluctuation forces of the thermal nature obey statistical laws, it is more correct to call the respective defect stability criterion probabilistic-energetic one.

As shown in [4–6, 8, 19, 44, 45], transformation of a defect is a sequence of elementary acts of detachment and displacement of dislocations, decay of defect clusters, and diffusion of ions. In turn, each elementary act is a change in the state of one of the particles that make up the defect. The elementary acts are thermally activated and characterized by the activation energy E_a. This means that an elementary act of the defect transformation requires initiating thermal energy, causing a fluctuation in the particle energy equal to E_a.

From the viewpoint of the probability theory, the elementary acts may be considered as random events that are characterized by a random variable – the time before a fluctuation of the particle energy by the value E_a [44, 45]. This time is characterized by a distribution function $F(t)$ [44, 45]:

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

where τ is the average time until the particle energy fluctuates with the value E_a:

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

Here, τ_0 is the pre-exponential factor, which by the order of magnitude coincides with the thermal oscillations period of the particle in the semiconductor lattice.

The probability-energetic criterion of defect stability in semiconductor crystals to action of external fields is formulated as follows [45]. Transformation of a defect is possible if the energy of the field localized in its volume V is equivalent to such kT value that an energy fluctuation by E_a is ensured at least for one particle of the defect to change its state for the time t of the field action.

Mathematically, the probability-energetic criterion of defect stability to action of external fields is written in the following form [7]:

$$w_{th} = \frac{E_a}{V \ln\left(\frac{VNt}{\tau_0}\right)}, \quad (3)$$

where w_{th} is the threshold (minimum) value of the volumetric energy density of the external field, at which stability of a defect of the volume V is lost, and VN is the number of the particles in the defect (N is the concentration of the particles), respectively.

Below, there is a summary of formulas for the threshold values of constant magnetic flux density B_{th} and the amplitude values of the electric E_{mth} and magnetic B_{mth} components of an electromagnetic wave, at which loss of stability of defects in semiconductor structures is observed [45]:

$$B_{th} = \left[\frac{2\mu\mu_0 E_a}{V \ln(VNt/\tau_0)}\right]^{1/2}, \quad (4)$$

$$B_{mth} = \left[\frac{2\mu\mu_0 E_a}{V \ln(VNt/\tau_0)}\right]^{1/2}, \quad (5)$$

$$E_{mth} = \left[\frac{2 E_a}{\varepsilon\varepsilon_0 V \ln(VNt/\tau_0)}\right]^{1/2}. \quad (6)$$

Here, μ is the magnetic permeability of the semiconductor, ε is the permittivity of the crystal, μ_0 is the magnetic constant, and ε_0 is the electric constant, respectively. Therefore, each defect can be assigned a certain threshold value of an external field parameter that causes its transformation.

In particular, the probability-energetic criterion predicts [45] the following experimentally observed patterns of the changes of magnetically sensitive quantities in semiconductor structures under influence of a magnetic field [6, 8]: presence of threshold values of magnetic flux density, saturation effects in the changes of the characteristics of materials, and quadratic dependence of the observed phenomena.

In [45], the threshold values B_{th} equal to $4.7\cdot10^{-2}$ and $4.6\cdot10^{-2}$ T are estimated for edge dislocations with a length of 10^{-6} m and a core radius equal to two lattice parameters, as well as for defect clusters in the form of a sphere with a radius of 10^{-8} m, respectively, in GaAs crystals subjected to the action of a magnetic field during 60 s. The obtained results are consistent with the values of the magnetic flux density obtained in the study of long-term non-monotonic changes in the intensity of photoluminescence bands of GaAs stimulated by such field [5, 6, 8].

4. Mathematical foundations of physical-statistical analysis of defect structure reconstruction in semiconductors under action of magnetic and electromagnetic fields

As noted in the previous section, transformation of defects is caused by random events. A flow of random events causes a change in the concentrations of generated, annihilated and moved point and linear defects over time, *i.e.*, it determines occurrence of physical-chemical processes in semiconductor materials. Consequently, mathematical description of the random events will allow us to obtain analytical relationships for the time patterns of evolution of the semiconductor structure parameters caused by action of magnetic or electromagnetic fields [44].

The mathematical description of the corresponding random events implies finding the law of distribution of a random variable – time to the specified event. As noticed above, the analyzed events are random because they have a thermal activation nature, *i.e.* they are determined by such a random event as fluctuation of a given particle energy. Therefore, the distribution law of a random variable – time to each of the specified events – depends on whether the activation energy of the event is deterministic or a random variable for the entire set of events [44].

First, let us consider the situation when the activation energy for each event from the entire set of the events has the same value E_a, *i.e.*, is a deterministic value. In this case, the time distribution function $F(t)$ before the event coincides with the time distribution function (1) before fluctuation of the particle energy by the value E_a [44].

Let us analyze the case when the activation energy of an event is a random variable for the entire set of the events. The type of the distribution function of the time to the event $F(t)$ is determined by the B.V. Gnedenko's theorem [44]. As applied to the analyzed situation, it is formulated as follows [44]. Let us consider a sequence of n independent random variables $t_1, t_2, ..., t_n$, which are the times to the events with the activation energies $E_{a1}, E_{a2}, ..., E_{an}$. Hence, n is the total number of events. Distribution of each of the random variables $t_1, t_2, ..., t_n$ is a distribution of the form (1) with $m = 1$, in which the variable E_a takes the values $E_{a1}, E_{a2}, ..., E_{an}$. We introduce a new value $\xi_n = \min(t_1, t_2, ..., t_n)$. The limiting distribution of the minimum value is called the Weibull–Gnedenko distribution. The corresponding function has the following form [44]:

$$F(t) = 1 - \exp\left[-\left(\frac{t}{\tau}\right)^m\right], \tag{7}$$

where m is the distribution form parameter and τ is the scale parameter, which we will call the time constant of a random event. Therefore, just as the equation of motion of a physical system is derived from the least-action principle, the evolution of a non-equilibrium state of defects in a semiconductor crystal is described by a distribution function of a random variable, which is the minimum of a large number of independently acting variables [44].

The distribution (1) is a special case of (7), in which $m = 1$ and τ is the average time (2) until the particle energy fluctuates by the value E_a. It is called an exponential distribution.

In turn, the dynamics of change of any parameter $\alpha(t)$ of a semiconductor structure sensitive to the action of magnetic or electromagnetic fields is proportional to (7) and is described by the following expression [44]:

$$\alpha(t) = \alpha_{in} + \alpha_0\left\{1 - \exp\left[-\left(\frac{t}{\tau}\right)^m\right]\right\}, \tag{8}$$

where α_{in} is the value of the parameter $\alpha(t)$ at the initial moment of time and α_0 is the proportionality coefficient such that $\alpha_0 = \alpha(t \to \infty) - \alpha_{in}$, respectively.

5. Physical-statistical modeling of time transformations of radiative recombination spectra due to action of microwave radiation and magnetic fields

We apply the theoretical concepts derived in Section 4 for physical-statistical modeling of time transformations of the intensity of integrated edge and impurity photoluminescence bands of n-GaAs and n-GaN epitaxial structures after treatments with 2.45 GHz microwave radiation and a pulsed magnetic field with the amplitude induction of 60 mT [4, 5, 8, 19]. It was shown that the evolution of the photoluminescence spectra is caused by rearrangement of defects in the near-surface regions of the studied semiconductor structures (the near-surface region should be understood as the region, in which electron-hole pairs are generated by photoluminescence excitation light) [4, 5, 8, 19].

- The following random events are introduced. Random events of the first type: defect migration from the near-surface region or generation (annihilation) of a defect in it.
- Random events of the second type: defect migration to the near-surface region or annihilation (generation) of a defect in this region.

Then the random variable represents the time until a random event. Accordingly, $F_1(t)$ is the distribution function of the time until any of the events of the first type (event probability), and $F_2(t)$ is the distribution function of the time until any of the events of the second type.

Table 1. Fitted parameters for the expression (10).

Fitted parameter	Magnetic field treatment				Microwave radiation treatment			
	GaN:Si	InP:Te	GaAs:Te	GaP:Te	GaN/Al_2O_3		n-n^+-GaAs	
					Edge emission	Impurity emission	Edge emission	Impurity emission
I_0	–0.36	–0.98	2.74	4.51	1.92	6.22	3.1	2.46
τ_1 (days)	9.68	19.02	10.02	13.01	7.03	6.99	5.62	5.8
τ_2 (days)	21.01	26.11	29.03	20.02	8.02	8.05	95.01	90.08
m_1	1.32	1.11	2.05	11.21	3.15	5.02	1.74	1.51
m_2	2.74	12.01	2.37	3.74	6.94	7.08	0.87	1.10

Without limiting the generality, we will assume that the event of the first type is the migration of a defect from the near-surface region, and the event of the second type is the migration of a defect to the near-surface region.

Let us consider a new random event – absence of a defect in the near-surface region. This event is complex and consists of a random event – the defect moving from the near-surface region, and a random event –absence of a defect moving to the near-surface region. We will consider these events to be independent. The probability $P(t)$ of this complex event is equal to the product of the probabilities of the component events [4, 5, 8, 19]:

$$P(t) = F_1(t)[1 - F_2(t)]. \tag{9}$$

By $F_1(t)$ and $F_2(t)$, we mean the Weibull–Gnedenko distribution functions of the form (7). According to (8), the integrated photoluminescence intensity $I(t)$ is expressed as follows [4, 5, 8, 19]:

$$I(t) = I_{in} + I_0\left\{\left[1 - e^{-(t/\tau_1)^{m_1}}\right]e^{-(t/\tau_2)^{m_2}}\right\}, \tag{10}$$

where I_{in} is the initial photoluminescence intensity, I_0 is the proportionality coefficient, τ_1 and τ_2 are the time constants of the random events, and m_1 and m_2 are the form factors, respectively. Table 1 presents the results of the least-squares approximation by expression (10) of the change in the integrated photoluminescence intensity of the edge and impurity bands for III-V compounds [4, 5, 46]. This approach made it possible to obtain good agreement between the experimental and theoretical results, which indicates the effectiveness of the performed physical-statistical modeling [4, 5, 46].

6. Physical-statistical modeling of photoluminescence spectra transformations stimulated by magnetic field treatments based on the mass service theory concepts

Probabilistic concepts can be effectively used to analyze the physical nature of phenomena in semiconductors caused by action of external fields. Let us demonstrate this by using an example of temporal behavior of photoluminescence spectra after the action of magnetic fields on a semiconductor.

It was shown in [47] that long-term changes in the photoluminescence spectra of n-GaN semiconductor structures after treatment in a pulsed magnetic field reveal the following important feature. In the analyzed structures, two photoluminescence bands were present: an edge band near 3.4 eV and an impurity band near 2.2 eV, the origin of which was associated with the presence of defects (donors and acceptors) in the semiconductor. After treatment in a pulsed magnetic field, long-term non-monotonic changes in the intensity of the photoluminescence bands were observed. At this, the intensity of the donor-acceptor photoluminescence remained virtually unchanged, while the intensity of the edge photoluminescence significantly decreased.

Such features of the behavior of the edge and donor-acceptor photoluminescence can be explained by assuming that restructuring of the defect subsystem in the near-surface region of the semiconductor takes place due to pulsed magnetic field treatment, which stimulates formation of additional donor levels in the material band gap, *i.e.*, the number of the donor levels becomes greater than the number of the acceptor levels [47]. Since the lifetime of non-equilibrium charge carriers for interband radiative recombination in n-GaN is longer than that for donor-acceptor radiative recombination, a queue of non-equilibrium electrons at the donor levels is formed, awaiting freeing the recombination channels with holes at the acceptor levels. Since these electrons do not participate in the edge photoluminescence, its intensity decreases. Since the number of the donor-acceptor pairs does not change due to the constancy of the number of the acceptor levels, the intensity of impurity recombination does not change as well.

From the viewpoint of the probability theory, this ensemble of the donor and acceptor energy levels in the band gap of n-GaN can be considered as a multi-channel system of mass queuing of donor-acceptor radiative recombination. Operation of a mass queuing system consists in servicing the flow of the requests coming into it. By requests we mean non-equilibrium electrons captured by the donor levels. Servicing of a request is the recombination of an electron at a donor level with a hole at an acceptor level. Finally, the servicing channels are pairs of donor-acceptor levels in the band gap of the semiconductor. This system of mass queuing of donor-acceptor radiative recombination is a system with waiting, since non-equilibrium electrons at the donor levels, having found all the recombination channels occupied, stand in a queue and wait until some channel becomes free. The length of the queue is equal to the difference in the numbers of the donor and acceptor levels.

The probability of queue formation is

$$P_Q = \frac{\rho^n}{n!} \times \frac{1-(\rho/n)^m}{1-(\rho/n)} P_0 , \quad (11)$$

where $\rho = \lambda/\mu$, λ is the average number of non-equilibrium electrons captured by the donor levels per unit time, μ is the average number of non-equilibrium electrons that annihilate with holes per unit time, n is the number of the recombination channels equal to the number of the acceptor levels, m is the number of non-equilibrium electrons in the queue at the donor levels, and P_0 is the probability of system downtime when all the system channels are free, equal to

$$P_Q = \left\{ \sum_{k=0}^{n} \frac{\rho^k}{k!} + \frac{\rho^{n+1}}{n!(n-p)} \left[1 - \left(\frac{\rho}{n} \right)^m \right] \right\}^{-1} . \quad (12)$$

The calculations presented show that $P_0 \approx 0$, and $P_Q \approx 1$, *i.e.* confirm formation of queues of non-equilibrium charge carriers. Therefore, the observed physical picture of the transformation of photoluminescence spectra of *n*-GaN due to magnetic field treatments in individual cases can be interpreted from the viewpoint of the concepts of mass queuing theory [47].

7. Deterministic and stochastic principles of the mechanisms of reactions of defects in semiconductor structures to action of magnetic and electromagnetic fields

7.1. Statistical features of the electroresonance mechanism of defect reconstruction under action of microwave radiation

Let us analyze the mechanisms of resonant detachment of dislocations and decay of clusters of impurity complexes in semiconductor crystals.

It is shown in [4, 6, 8] that electrically charged dislocations pinned at the ends have a natural angular frequency of oscillations ω_D equal to

$$\omega_D = \frac{\pi}{L} \left(\frac{G}{\rho_V} \right)^{\frac{1}{2}} , \quad (13)$$

where G is the Poisson ratio, ρ_V is the bulk density of the material, and L is the dislocation length, respectively.

When the electromagnetic radiation and the dislocation natural oscillation frequencies coincide, resonance phenomena are observed. At the resonance frequency, under the action of the electric component of the electromagnetic wave, the amplitude and, hence, the energy of the dislocation oscillations sharply increase, which leads to dislocation detachment and movement under the action of internal mechanical stress in the semiconductor crystal. This effect is characterized by strong selectivity by the lengths of the detached dislocations with respect to the frequency of the electro-magnetic radiation. In particular, for epitaxial structures of *n*-GaAs and *n*-GaN, at the carrier frequency of the microwave generator used in the experiments equal to 2.45 GHz, only dislocations with the lengths $L = 5.07 \cdot 10^{-7}$ and $6.73 \cdot 10^{-7}$ m, respectively, are detached [4, 6, 8].

However, the experimental picture is significantly changed by the fact that the resonator, in which semiconductor structures are placed, is characterized by a wide spectrum of excited electromagnetic oscillations relative to the carrier frequency of the magnetron [6, 8]. The probabilistic distribution of the frequencies of electromagnetic oscillations in the resonator complements the deterministic law of electrical resonance with respect to the behavior of dislocation systems in semiconductor crystals. One may say that the resonant effect at a given carrier frequency of the magnetron is no more selective but covers an ensemble of defects with different resonant frequencies.

As a consequence, resonant detachment of dislocations with a wide range of lengths becomes possible. Therefore, dislocations with the lengths L that satisfy the conditions [6, 8]: $L \le 4.05 \cdot 10^{-6}$ m and $\le 5.4 \cdot 10^{-6}$ m for *n*-GaAs and *n*-GaN, respectively, are subject to transformations. Probabilistic distribution of the frequencies of electromagnetic oscillations in the resonator is the reason that use of a different carrier frequency of the microwave radiation generator in experiments leads to a similar defect behavior.

Let us analyze the decay of defect complexes in semiconductor structures under action of microwave radiation. In *n*-GaAs crystals containing copper impurity, impurity complexes – donor-acceptor pairs $Cu_{Ga}^{-}Te_{As}^{+}$ – may form. In turn, these donor-acceptor pairs are capable of combining into electrically neutral clusters [4, 6, 8]. For these clusters, the frequency of ion-plasma oscillations is equal to [4, 6, 8]

$$\omega_P = \left(\frac{e^2 N_i}{\varepsilon \varepsilon_0 \mu} \right)^{\frac{1}{2}} , \quad (14)$$

where e is the electron charge, N_i is the concentration of copper and tellurium ions in the cluster, and μ is the reduced mass of an ion pair, respectively.

Coincidence of the frequency of the microwave radiation with the ion-plasma frequency induces resonant increase in the amplitude of ion oscillations and decay of the impurity complexes, and, consequently, of the clusters consisting of them, followed by diffusion of charged point defects.

The calculations for *n*-GaAs epitaxial structures performed in [4, 6, 8] give $\nu_P = \omega_P/2\pi = 2.01$ GHz. The obtained value is close to 2.45 GHz, the carrier frequency of the microwave generator used in the experiments.

As was already noted, electromagnetic oscillations in the resonator have a wide range of frequencies. Statistical distribution of the frequencies of electromagnetic oscillations excited in the resonator complements the deterministic patterns of resonant oscillations of ions in the clusters. As a consequence, resonant decay of the analyzed clusters of impurity-defect complexes becomes possible.

7.2. Statistical regularities of the electroresonance mechanism of defect transformation caused by action of pulsed magnetic fields

In a magnetic field, mobile charge carriers in semiconductor structures emit electromagnetic waves at the cyclotron frequency during their rotation [5, 6, 19]. In particular, under action of a pulsed magnetic field with an amplitude induction of 60 mT, conduction electrons in *n*-GaAs and *n*-GaN generate electromagnetic waves at the cyclotron frequencies of 27 and 8.4 GHz, respectively [5, 6, 19]. Electromagnetic radiation causes defect reconstruction according to the electroresonance mechanisms discussed in Section 7.1.

The deterministic-stochastic nature of the mechanism of defect reconstruction under action of pulsed magnetic fields is as follows. The spectral lines of cyclotron radiation of electrons in a semiconductor crystal are not infinitely narrow, since charged carriers moving under the action of a magnetic field are scattered by phonons and defects. This leads to broadening of the cyclotron radiation line in both directions relative to the cyclotron frequency. The generated pulsed magnetic field contains rising and falling segments of the magnetic flux density [5, 6, 19], in which its magnitude is much lower than the amplitude value. Hence, the cyclotron frequency will be lower than the values given above.

Consequently, electromagnetic oscillations in a wide frequency spectrum will be generated in a semiconductor crystal, including the frequencies equal to the resonant oscillation frequencies of dislocations and clusters consisting of defect complexes [6, 19]. This means that the laws of evolution of magnetosensitive characteristics of materials under the action of fields with different deterministic amplitude values of magnetic induction are similar. The electroresonance mechanism of defect transformations under action of pulsed magnetic fields provides a rationale for the observed behavior of the magnetosensitive parameters with respect to magnetic flux density, including quadratic dependence, threshold effect and saturation effect [6, 19].

7.3. Stochastic resonance of point defects

Along with the resonance analyzed above, which is a physical phenomenon caused by deterministic behavior of a system, a resonance caused by non-deterministic (stochastic) dynamics – stochastic resonance – is also possible. In [48], this stochastic phenomenon was analyzed for semiconductor compounds A^3B^5 with covalent polar bonds between the atoms.

In the initial state, point defects (atoms, ions) are in local minima of double potential wells. When a semiconductor structure is exposed to an ultra-high-frequency radiation or a pulsed magnetic field, the periodic electric component of the electromagnetic field interacts with the effective charges of the atoms and deforms the potential of the double well. At small amplitudes of the electric component of electromagnetic oscillations, the change in the potential barrier height is insufficient for a particle to overcome the potential barrier with subsequent transition from one local minimum to another.

However, the situation becomes different when the particles in the symmetric double well are subject to thermal fluctuations. Under certain conditions, these fluctuations lead to stimulation of jumps between the minima of the symmetric double potential well at the frequency of the weak periodic action at the moments of the peak values of the latter. This statistical synchronization is called stochastic resonance.

The expression for the frequency ω_S of the stochastic resonance of point defects has the following form [48]:

$$\omega_S = \pi \nu_0 \exp\left(-\frac{U_0}{kT}\right), \qquad (15)$$

where U_0 is the height of the potential barrier separating the local minima and ν_0 is the frequency factor, which by the order of magnitude coincides with the frequency of thermal oscillations of the particle. In particular, at $U_0 = 0.2$ eV, the frequency of stochastic resonance of defects is $\nu_S = 1.3$ GHz [48].

The picture of stochastic resonance of point defects is supplemented by the above-mentioned factor of statistical distribution of frequencies of electromagnetic fields under action of pulsed magnetic fields and microwave radiation on a semiconductor structure. As a consequence, this mechanism can be inherent in point defects with a wide range of resonant oscillation frequencies.

7.4. Deterministic and stochastic aspects of drift phenomena of charged point defects under action of electromagnetic and magnetic fields

Let us analyze the features of drift of charged point defects (ions) in semiconductor structures under action of a uniform microwave field.

It is shown in [49] that singly charged point defects drift in an electromagnetic field with a velocity υ_E equal to

$$\upsilon_E = -\frac{eE_0 \sin\varphi}{m_{eff}\,\omega}, \qquad (16)$$

where E_0 is the amplitude of the electric component of the electromagnetic field, ω is the circular frequency of the field, φ is the phase of the field at the initial moment of time, $m_{eff} = m\exp(E_a/kT)$ is the effective mass of the impurity ion that overcomes the potential barriers E_a during its movement in the semiconductor crystal, and m is the mass of the free ion, respectively.

As follows from (16), at $\sin\varphi = 0$, there is no directed motion of the ion, and for all other values of the phase φ, the charged point defect moves along the electric field. Depending on the φ values (sign of $\sin\varphi$), the charged particles drift in mutually opposite directions.

The stochastic feature of the noted drift phenomena is as follows. Since the initial phase φ is a random variable that obeys a continuous uniform distribution for the entire set of the charged point defects, the drift velocity of the defect ensemble averaged over φ is equal to zero. Therefore, the deterministic-stochastic regularity of the ion drift phenomena in a homogeneous ultra-high-frequency electromagnetic wave is that there is no directed movement of the entire set of particles as a whole together with the drift of individual charged defects.

In [49], the drift velocity values υ_E of singly charged copper ions in semiconductor structures subjected to action of a uniform microwave field are estimated for ν = 2.45 GHz, $E_0 = 1.5\cdot 10^3$ V/m, and $\varphi = -\pi/2$. At E_a = 0.4 eV, the drift velocity is $\upsilon_E = 0.28\cdot 10^{-7}$ m/s, and at E_a = 0.45 eV, we obtain $\upsilon_1 = 0.41\cdot 10^{-8}$ m/s, *i.e.* the drift velocity is highly sensitive to E_a.

Under an action of an alternating magnetic field, a vortex electric field is excited in a semiconductor structure. In this field, charged point defects drift with an azimuthal velocity υ_B, which is expressed as follows [50]:

$$\upsilon_B = \frac{S}{l}\frac{qB_0}{m_{eff}}\cos\varphi\,, \qquad (17)$$

where B_0 is the amplitude value of the magnetic induction, ω is the angular frequency of the induction change, φ is the initial phase, S is the surface area of the semiconductor structure, and l is the perimeter (length) of a contour limiting the surface, respectively. Drift of charged point defects is absent at initial phase values such that cos φ = 0 and occurs for all other values of the phase φ. Depending on the φ values, the particles drift in mutually opposite directions.

The deterministic-stochastic feature of the ion drift phenomena in an alternating magnetic field is as follows. Since the initial phase φ for the entire set of the charged point defects is a random variable that obeys a continuous uniform distribution, the drift velocity of the defect ensemble averaged over φ is zero. This means that there is generally no directed movement of the entire set of particles as a whole together with the drift of individual charged particles.

In [50], the drift velocity values υ_B of singly charged copper ions in semiconductor structures with the square surface having a side length of $4\cdot 10^{-3}$ m under the action of an alternating magnetic field are estimated at E_a = 0.4 eV and φ = 0. At $B_0 = 3\cdot 10^{-3}$ T, the drift velocity $\upsilon_B = 8.7\cdot 10^{-7}$ m/s, and at $B_0 = 3\cdot 10^{-2}$ T, we have $\upsilon_B = 8.7\cdot 10^{-6}$ m/s.

8. Conclusions

The physical-statistical approach to the analysis of the influence of external factors, including pulsed magnetic fields and microwave radiation, on transformation of the defect subsystem of semiconductor structures is based on the idea that evolution of this subsystem and the mechanisms causing it obey not only deterministic, *i.e.*, physical laws, but also statistical laws.

The constituent elements of the probabilistic-physical method for studying the defect transformations in semiconductor structures stimulated by action of external fields are: the probabilistic-energetic concept of defect stability to the action of the external fields; physical-statistical modeling of the laws of evolution of the defect subsystem of semiconductor structures under the influence of a magnetic field and microwave radiation; and deterministic-stochastic nature of the mechanisms of defect reconstruction under the action of a magnetic field and microwave radiation.

The methodology of the physical-statistical analysis of reactions of a defect subsystem of semiconductors to external influences allows one to explain the experimentally observed regularities such as similarity of the evolution of the characteristics of materials under external influences at different deterministic values of the indicators of force fields, presence of threshold values of the parameters of the fields, and saturation of changes of the characteristics of materials and quadratic dependence of the observed phenomena.

The probability-energetic criterion of defect stability in semiconductor crystals allows estimating the potential stability of defects to the action of external fields. The essence of the criterion is that to change the state of a defect, the field energy localized in its bulk must be equivalent to such kT value, at which at least one particle of the defect will experience an energy fluctuation sufficient to change its state during the action of the field. Therefore, each defect has a threshold (minimum) value of the parameter characterizing the external field, upon reaching which its transformation takes place. This criterion allows explaining the experimentally observed regularities of the magnetic field treatments: presence of threshold values of magnetic field induction, saturation effects in changes in the characteristics of materials and the quadratic dependence of the observed phenomena.

The mathematical foundations of the physical-statistical analysis of the time regularities of reconstruction of the defect structure of semiconductors under action of magnetic and electromagnetic fields are based on the following concepts: (i) the elementary acts of defect transformation are random events, the mathematical description of which implies finding the distribution function of a random variable – time before the specified event; (ii) the dynamics of change in time of any parameter of a semiconductor structure sensitive to the action of magnetic or electromagnetic fields is proportional to this function; (iii) just as the equation of motion of a physical system is derived from the least-action principle, evolution in time of a defect subsystem in a semiconductor crystal under the action of external fields is described by a distribution function of a random variable, which is the minimum of a large number of independently acting values. The extreme distribution of the minimum values is the Weibull–Gnedenko distribution. Physical-statistical modeling of time transformations of the integrated photoluminescence intensity of epitaxial structures shows good agreement between the experimental and theoretical results.

The evolution of the defect subsystem of semiconductor structures due to action of pulsed magnetic fields and microwave radiation is based on general mechanisms including resonance and drift phenomena. The possible types of resonance are electrical resonance of charged dislocations followed by their detachment and migration under the action of the internal mechanical stress in the semiconductor crystal, and electrical resonance of clusters of impurity complexes of defects followed by their decay and diffusion of the decay products. Along with the electrical resonance, which is a physical phenomenon caused by deterministic behavior of the system, the resonance caused by non-deterministic (stochastic) dynamics – stochastic resonance of point defects – is also possible.

The essence of the latter is that under certain conditions, particle jumps under the action of thermal fluctuations between the minima of a symmetric double potential well, which are elementary acts of the defect transformation, occur at the frequency of a weak periodic electrical action at the moments of the peak values of the latter. The picture of the electrical and stochastic resonances is supplemented by the factor of statistical distribution of electromagnetic field frequencies under an action of pulsed magnetic fields and microwave radiation on a semiconductor structure.

Consequently, these mechanisms are the cause of transformations of point defects, their clusters, and linear defects with a wide range of resonance oscillation frequency values. This means that under action of fields with different deterministic values of force characteristics, the laws of evolution of material parameters sensitive to these fields show a similar picture. An important feature of the resonance phenomena is that even at small amplitude values of the force field parameters, the response of the defect subsystem at the resonance frequency is very significant.

All the observed mechanisms associated with modification of the defect composition should be considered in the development of next-generation thin-film solar cells.

Acknowledgment

This work was supported by the NATO SPS project G6197 "Plasmonically Enhanced Perovskite Thin-Film Solar Cells" and by the National Academy of Sciences of Ukraine (Project No. 4.11/23-P).

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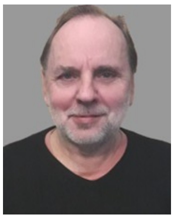

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Фізико-статистичні основи аналізу трансформації дефектів у напівпровідникових структурах під дією магнітних та електромагнітних полів

Г.В. Міленін, Р.А. Редько

Анотація. У статті представлено методику фізико-статистичного аналізу трансформації дефектів у напівпровідникових структурах під дією магнітних та електромагнітних полів. Проаналізовано ймовірнісно-енергетичний критерій стабільності дефектів до зовнішніх полів. Сформульовано математичні основи фізичного та статистичного аналізу перебудови дефектної структури напівпровідників під дією магнітних та електромагнітних полів. Проведено ймовірнісно-фізичне дослідження часових перетворень спектрів радіаційної рекомбінації внаслідок дії мікрохвильового випромінювання та обробки магнітним полем. Розглянуто механізми перебудови дефектів у напівпровідниках під впливом магнітних та електромагнітних полів.

Ключові слова: точковий дефект, дислокація, кластер дефектів, магнітне поле, мікрохвильове випромінювання.