

Transformation of defects in semiconductor structures under action of magnetic fields stimulated by drift phenomena

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Abstract. The phenomenon of directed motion of mobile charged point defects in semiconductor structures under action of magnetic fields has been discussed. The features of defect drift in sign-changing magnetic fields have been studied. The effect of directional movement of charged defects under the combined action of constant and alternating magnetic fields has been analyzed. Analytical relations have been presented for the drift rate of defects in semiconductor structures under given impacts.

Keywords: magnetic field, charged defect, defect drift.

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1. Introduction

In [1–12], the mechanisms of transformation of defects in semiconductor structures under action of weak magnetic fields were considered. They are based on the concept of the occurrence of spin-dependent reactions (singlet-triplet transitions), magnetic and electrical resonance phenomena in systems of crystal defects: dislocations and clusters of impurity-defect complexes. The universality of the electrical-resonance mechanism of transformation of a defect structure in epitaxial semiconductor films both under action of alternating, in particular pulsed magnetic fields, and under action of microwave radiation was noted in [11, 12].

At the same time, it should be noted that, in addition to the above, other reasons for evolution of defects under action of alternating magnetic fields cannot be excluded. They may be based on the idea that an alternating magnetic field induces a vortex electric field. In its turn, in an alternating electric field, charged particles not only oscillate, but their directed movement is also possible [13], and, consequently, a directed movement of charged point defects (ions) takes place [14].

This paper is devoted to studying the mechanisms of drift of mobile charged point defects in semiconductor crystals under action of magnetic fields.

2. Drift of mobile charged point defects in a semiconductor structure under action of an alternating magnetic field

Let the change in the induction of alternating magnetic field acting on a semiconductor structure be described by a periodic function:

$$B = B_0 \cos(\omega t + \varphi), \quad (1)$$

where B_0 is the amplitude value of the magnetic induction, ω – angular frequency of induction change, φ – initial phase.

An alternating magnetic field excites a vortex electric field in the semiconductor. The electromotive force of electromagnetic induction has the form [15]:

$$\varepsilon = -\frac{d\Phi}{dt}, \quad (2)$$

where Φ is the flux of the magnetic induction vector \vec{B} through the surface of the semiconductor structure \vec{S} , which, in turn, is equal to [15]:

$$\Phi = \int_S \vec{B} \cdot d\vec{S}. \quad (3)$$

If the magnetic field induction B is not a function of the coordinate, that is, at an arbitrary moment of time it is constant at any point of the surface with the S area (uniform magnetic field), then

$$\Phi = BS \cos \alpha, \quad (4)$$

where α is the angle between the magnetic induction vector and the normal to the surface.

At $\alpha = 0$, the electromotive force of electromagnetic induction (2) is equal to:

$$\varepsilon = -S \frac{dB}{dt}. \quad (5)$$

The circulation of the strength vector of the vortex electric field \vec{E} along the contour \vec{l} , on which the surface with the area S is supported, is described by the relation [15]:

$$\oint \vec{E} d\vec{l} = \varepsilon. \quad (6)$$

Since at an arbitrary moment of time the magnetic induction B is constant at any point of the surface with the area S , then the strength of the vortex electric field E at any point of the contour with the length l (uniform electric field) that limits this surface will also be constant, and therefore:

$$E = \frac{\varepsilon}{l}. \quad (7)$$

From (5) and (7), it follows that

$$E = -\frac{S}{l} \frac{dB}{dt}. \quad (8)$$

In a particular case, when the surface of a semiconductor epitaxial film is a square with the side a , then the ratio of the surface area to its perimeter is $S/l = a/4$.

Taking into account (1) and (8), we obtain an expression for the strength of the vortex electric field in a semiconductor crystal:

$$E = E_0 \sin(\omega t + \varphi), \quad (9)$$

moreover, the amplitude value of the electric field strength E_0 is:

$$E_0 = \frac{S}{l} B_0 \omega. \quad (10)$$

If the magnetic induction vector is directed along the z -axis of the Cartesian coordinate system, then the vortex electric field is located in the x - y plane. The force lines of this field are closed. Since the electric field is uniform, its force lines are circles. Therefore, to describe the dynamics of charged point defects in such a field, it is expedient to use the polar coordinate system. In a polar coordinate system, the position of a particle is characterized by a polar radius r and polar angle (azimuth) ϕ .

Since there is no movement of ions along the radius, then Newton's Second Law for a charged particle is written as follows:

$$m_{eff} r \frac{d^2 \phi}{dt^2} = qE_0 \sin(\omega t + \varphi), \quad (11)$$

moreover, since the movement of ions with a charge q in semiconductor crystals is of a thermally activated nature, that is, when moving, they have to overcome potential barriers with a height of E_a , then the mass of the particle means the effective mass [14] $m_{eff} = m \exp(E_a/kT)$, where m is the mass of the free ion, k – Boltzmann's constant, T – absolute temperature.

Integrating (11) and taking into account (10), we obtain the relation for the azimuth velocity expressed in coordinates (hereinafter referred to as the azimuth velocity):

$$r \frac{d\phi}{dt} = -\frac{S}{l} \frac{qB_0}{m_{eff}} \cos(\omega t + \varphi) + C, \quad (12)$$

where C is the integration constant determined from the initial condition.

Assuming that at the initial moment of time $t = 0$ the particle is at rest, that is, its azimuthal velocity $r d\phi/dt = 0$, we have the expression for C :

$$C = \frac{S}{l} \frac{qB_0}{m_{eff}} \cos \varphi. \quad (13)$$

Then for the azimuth velocity we get:

$$r \frac{d\phi}{dt} = \frac{S}{l} \frac{qB_0}{m_{eff}} [-\cos(\omega t + \varphi) + \cos \varphi]. \quad (14)$$

The first term in square brackets characterizes the oscillatory motion of a charged point defect, and the second one, independent of time, characterizes the directed motion (drift). Thus, for the azimuthal drift velocity v_1 (hereinafter referred to as drift velocity), we can write:

$$v_1 = \frac{S}{l} \frac{qB_0}{m_{eff}} \cos \varphi. \quad (15)$$

In general, the obtained results agree with the conclusions presented in [13] and [14]. In [13], the justification was given for the directed motion of charged particles in space under action of electric field that is sign-changing, uniform and directed along one coordinate. In [14], a similar problem was considered for mobile charged point defects (ions) of a semiconductor structure.

At the same time, a feature of Exp. (15) is the absence of a dependence of the drift velocity on the frequency of change in the magnetic field, and hence in the vortex electric field (for an electric sign-changing field, an inversely proportional dependence of the velocity on frequency takes place [13, 14]). In addition,

the drift velocity of charged point defects is directly proportional to the amplitude value of the magnetic induction (in the case of an alternating electric field, it is proportional to the amplitude value of its strength) and inversely proportional to the effective mass of ions. Finally, an important distinguishing feature of the motion of charged point defects in a sign-changing magnetic field is the dependence of the drift velocity on the geometric dimensions of the semiconductor structure, namely, the ratio of its surface area to the perimeter (geometric size effect).

It follows from (15) that there is no drift of charged point defects at the values of the initial phase such that when $\cos\varphi = 0$, and for all other values of the phase φ it takes place, and depending on the φ values, the particles drift in mutually opposite directions. The absolute maximum value of the drift velocity $|v_1|_{\max}$ takes place at $\varphi = 0$ and π . It satisfies the relation:

$$|v_1|_{\max} = \frac{S}{l} \frac{qB_0}{m_{eff}}. \quad (16)$$

It should be noted that for the entire set of charged point defects, the initial phase φ is a random value that obeys a continuous uniform distribution. In its turn, since all the values of initial phase are equally probable, the drift velocity averaged over φ is equal to zero. It means that along with the systematic movement of individual charged particles, in general, directed movement of the entire set of particles is absent [13, 14].

3. Drift of mobile charged point defects in a semiconductor structure under combined action of constant and alternating magnetic fields

Let us consider motion of a charged point defect in a combined magnetic field with both constant and variable parallel oriented components:

$$B = B_C + B_0 \cos\omega t, \quad (17)$$

where B_C is the induction of magnetic field.

As shown in the previous section, in a sign-changing magnetic field the drift of charged point defects is observed. In its turn, in a constant magnetic field, the motion of a charged particle is finite, and directed motion is not observed on average over time. However, in a combined magnetic field the drift phenomena are also possible, but when a certain condition is satisfied.

In a combined magnetic field, the movement of ions in the x - y plane normal to the magnetic induction vector in the case of very low attenuation obeys the system of equations [16]:

$$\frac{dx}{dt} = f + \Omega y, \quad \frac{dy}{dt} = -\Omega x, \quad f = \frac{qE}{m_{eff}}, \quad \Omega = \frac{qB}{m_{eff}}, \quad (18)$$

where the electric field is defined by (8).

Special solutions of this system of equations describe the phenomenon of parametric resonance. This

resonance is observed when the frequency ω of the variable component of the magnetic field is either equal to the cyclotron frequency of ion ω_{Bc} in the field with the induction B ($\omega_{Bc} = qB_C/m_{eff}$) or is its subharmonic [16].

Under the resonance conditions, the magnetic field B induces a constant component in the ion displacement. At $\omega = \omega_{Bc}$, the square of the drift velocity averaged over a large time interval is written as [16]:

$$\overline{v^2} = 2\omega_{B_0}^2 \left(\frac{S}{l}\right)^2 J_1^2\left(\frac{2B_0}{B_C}\right) \left(\frac{1}{2} + \omega t\right), \quad (19)$$

where $\omega_{B_0} = qB_0/m_{eff}$ is the cyclotron frequency of a particle in a magnetic field with the induction B , $J_1(2B_0/B_C)$ – Bessel function of the first kind of the first order.

In (19), the term ωt describes an unlimited increase in the drift velocity at the resonance, when there is no attenuation in the system. However, attenuation takes place in physical systems and is often significant, so that part of the drift velocity that depends on the magnetic field induction is of interest. Then we have [16]:

$$\overline{v^2} \approx \left(\frac{S}{l}\right)^2 \left(\frac{qB_0}{m_{eff}}\right)^2 J_1^2\left(\frac{2B_0}{B_C}\right), \quad (20)$$

where $\omega_{B_0} = qB_0/m_{eff}$ is the cyclotron frequency of a particle in a magnetic field with the induction B , $J_1(2B_0/B_C)$ – Bessel function of the first kind of the first order.

Accordingly, the value of the average squared drift velocity (hereinafter simply the drift velocity) v_2 is equal to $v_2 = \sqrt{\overline{v^2}}$. Taking into account (20), we obtain:

$$v_2 \approx \left| \frac{S}{l} \frac{qB_0}{m_{eff}} J_1\left(\frac{2B_0}{B_C}\right) \right|. \quad (21)$$

The sign of the modulus reflects the fact that the Bessel function takes both negative and positive values.

Thus, the drift velocity of charged point defects is inversely proportional to the effective mass of ions and directly proportional to the ratio of the surface area of the semiconductor structure to its perimeter (geometric size effect). From the geometric viewpoint, the parametric resonance is observed when the linear size of the semiconductor structure a is larger than the double cyclotron (Larmor) radius of the charged point defect R : $a > 2R$. Taking into account that $R = v_T/\omega_{Bc}$ with $v_T = \sqrt{3kT/m_{eff}}$ – average squared thermal velocity of ions, we get $a > 2\sqrt{3kTm_{eff}}/qB_C$.

The velocity of directional movement has a complex nonmonotonic dependence on the parameters of induction B_0 and B_C of the combined magnetic field. In a particular case, when $B_0 = B_C$ the drift velocity is

directly proportional to the value of the magnetic induction, as it is observed under action of only one variable field (11).

In absolute terms, the first extremum of the first-order Bessel function has the greatest value as compared to other values of the function over the entire interval of the argument changing. Approximate values of the parameters of this extremum are as follows: $B_0/B_C \approx 0.9$, $J(2B_0/B_C) \approx 0.58$. It follows that the maximum value of the drift velocity is

$$v_{2 \max} \approx 0.58 \frac{S q B_0}{l m_{\text{eff}}}, \quad (22)$$

which means that for any values of the parameters included to the expressions (16) and (22) the inequality will be fulfilled $v_{2 \max} < |v_1|_{\max}$.

The drift velocity becomes equal to zero at zero values of the Bessel function. The first zero of the Bessel function corresponds to the value of argument: $B_0/B_C \approx 1.9$.

Thus, the necessary conditions for the maximum velocity of directional movement of charged point defects is the fulfillment of the following requirements: $\omega = \omega_{B_C}$ and $B_0/B_C \approx 1.9$. It means that the largest change in the magnetically sensitive parameters of the semiconductor (parameters that depend on the change in the state of defects) will also be observed, if the specified requirements are met. Therefore, the method of varying the parameters of combined magnetic fields can be considered as a method for determining the effective mass of ions, and hence the activation energy of particle motion.

4. Calculation of the drift velocity of defects in semiconductor structures under action of an alternating magnetic field

Let us estimate the values of drift velocity v_1 for singly charged copper ions in epitaxial semiconductor structures, the surface of which is a square with a side $a = 4 \cdot 10^{-3}$ m under action of a sign-changing magnetic field with $B_0 = 3 \cdot 10^{-2}$ T. Taking into account that the mass of free copper ions is equal to $m = 1.055 \cdot 10^{-25}$ kg, then at $E_a = 0.4$ eV, $T = 300$ K and $\varphi = 0$, for the maximum drift velocity, calculation with the formula (15) gives the following value: $v_1 = 8.7 \cdot 10^{-7}$ m/s. At $E_a = 0.5$ eV and unchanged values of other parameters, we have $v_1 = 1.8 \cdot 10^{-8}$ m/s. At $B_0 = 3 \cdot 10^{-2}$ T, the corresponding velocity values are $v_1 = 8.7 \cdot 10^{-6}$ m/s and $v_1 = 1.8 \cdot 10^{-7}$ m/s. One can state the fact of sufficiently high velocities of directional movement of ions in sign-changing magnetic fields. This circumstance indicates the importance of the charged particle drift phenomenon considered in this work to explain transformation of defects in semiconductor structures in the corresponding magnetic fields.

5. Conclusions

Analyzed in this paper is the phenomenon of directional motion of mobile charged point defects in semiconductor structures under action of magnetic fields.

Under action of a sign-changing magnetic field on semiconductor, a directional movement of individual charged point defects in an induced vortex electric field is observed (in general, directional movement of the entire set of particles is absent). The drift velocity does not depend on the frequency of the field change, it is directly proportional to the amplitude value of the magnetic induction and inversely proportional to the effective mass of ions. In addition, an important feature of the movement of charged point defects in an alternating magnetic field is the dependence of the drift velocity on the geometric dimensions of the semiconductor structure, namely, the ratio of its surface area to the perimeter (geometric size effect).

In a combined magnetic field with both constant and variable components, drift occurs when the parametric resonance condition is satisfied: the frequency of the variable component of the magnetic field is equal to the cyclotron frequency of ion in a field with an induction equal to that of the constant component. The drift velocity of charged point defects, as in the previous case, is inversely proportional to the effective mass of ions and directly proportional to the ratio of the surface area of the semiconductor structure to its perimeter.

However, it has a nonmonotonic dependence on the induction parameters of the combined magnetic field. The drift velocity reaches a maximum or becomes equal to zero at such values of the ratio of inductions of the field components, which correspond to either the first extremum or zeros of the Bessel function. In the particular case of equality of inductions of the field components, the drift velocity is directly proportional to the magnetic induction over the entire range of its change, as it is observed under action of only one variable field.

The results obtained in this work are important to explain transformation of charged point defects in semiconductor structures under action of corresponding magnetic fields. In addition, since in combined fields the particle drift occurs at a certain (resonant) frequency, and its velocity depends nonmonotonically on the ratio of the magnetic inductions of the components, variation of the parameters inherent to these fields can be considered as a method for determining the effective mass of ions, and hence the activation energy of their migration.

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Milenin G.V.: conceptualization, writing – original draft, validation, writing – review & editing, methodology.

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Трансформація дефектів напівпровідникових структур під впливом магнітних полів, стимульована дрейфовими явищами

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Анотація. Розглянуто явище спрямованого руху рухомих заряджених точкових дефектів у напівпровідникових структурах при дії магнітних полів. Вивчено особливості дрейфу дефектів у знакозмінних магнітних полях. Проаналізовано ефект спрямованого переміщення заряджених дефектів при спільній дії постійного та змінного магнітних полів. Подано аналітичні співвідношення для швидкості дрейфу дефектів у напівпровідникових структурах при даних впливах.

Ключові слова: магнітне поле, заряджений дефект, дрейф дефектів.