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ОКРЕМІ АСПЕКТИ ТЕОРІЇ ВІДПАЛУ ДЕФЕКТІВ В ОПРОМІНЕНИХ КРИСТАЛАХ CdSb

Процеси утворення і перебудови радіаційних дефектів при опроміненні і відпалі можна розглядати як сукупність квазіхімічних реакцій різного порядку. Деякі із них важко звести до форми, яка б давала можливість проаналізувати часову залежність концентрації дефектів при відпалі.

Важливим параметром, який визначає кінетику відпалу дефектів, є енергія активації відпалу. Існує багато методів визначення цієї енергії. Ми користувалися методом перерізів, який ґрунтується на аналізі кривих Арреніуса при різних температурах відпалу. Для визначення області термостійкості радіаційних дефектів використовувалася методика ізохронного відпалу.

Ключові слова: *радіаційний дефект, опромінення, відпал, кристал CdSb, енергія активації, дифузія.*

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SOME ASPECTS OF THE THEORY OF DEFECT ANNEALING IN IRRADIATED CdSb CRYSTALS

The processes of formation and rearrangement of radiation defects during irradiation and annealing can be considered as a set of quasichemical reactions of different orders. Some of them are difficult to reduce to a form that would allow analyzing the time dependence of the defect concentration during annealing.

An important parameter that determines the kinetics of defect annealing is the annealing activation energy. There are many methods for determining this energy. We used the cross-section method, which is based on the analysis of Arrhenius curves at different annealing temperatures. To determine the thermal stability region of radiation defects, the isochronal annealing method was used.

Keywords: *radiation defect, irradiation, annealing, CdSb crystal, activation energy, diffusion.*

Statement of the problem. The annealing process is part of a complex of measurements to establish the nature and mechanisms of the physicochemical properties of materials. Theoretical approaches to annealing are based on the kinetics of defect reactions – diffusion of interstitial and vacancy components, their mutual recombination, or the formation of more stable complexes. Important concepts are defect mobility (diffusion coefficients), migration activation energies, charge carrier capture/emission by defects, and kinetic models of isochronal and isothermal annealing. The classical picture involves successive stages of annealing with increasing temperature – low-temperature recombination (mobile interstitial atoms), intermediate association (formation of complexes), and high-temperature reperforation (movement of vacancies/clusters). Mathematically, the processes are described by systems of diffusion-reaction equations or exponential relaxation laws with characteristic activation energies [1]. Theoretical aspects of semiconductor defect annealing have been analyzed in the literature [2-8].

Analysis of recent research and publications. In the modern semiconductor industry, there is a growing need to understand and combat potential radiation damage problems. Space applications are an obvious case, but, beyond that, today's device and circuit fabrication rely on increasing numbers of processing steps that involve an aggressive environment where inadvertant radiation damage can occur [3].

The authors [4] proposed and simulated the radiation defects type and amount of $Cd_{0.9}Zn_{0.1}Te$:In crystals after neutron irradiation with the Monte-Carlo software SRIM. The calculated data are also compared with experimental results of detector performance and the crystal defects obtained using thermally stimulated current (TSC) measurement. The effect of a fast neutron flux (Φ = 1014 – 1015 cm–2) on the electrical and photoluminescence properties of p-CdZnTe single crystals is studied [5]. Isothermal annealing is performed (T = 400 – 500 K), and the activation energy of the dissociation of radiation-induced defects is determined at ED ≈ 0.75 eV. The parameters that characterize process the annealing (the activation energies and frequency factors) of the main radiation defects in silicon (A-centers, E-centers, divacancies, etc.) have been ascertained, and various mechanisms and reactions that determine the conditions for the annealing of the defects were proposed [6].

It is revealed [7] that radiation defects of both donor and acceptor types are introduced into the lattice of the CdSb crystals with gamma-irradiation. The effectiveness of removal of carriers is a consequence of the involvement of impurity atoms in the formation of corresponding radiation defects with deep energy levels. Starting from the annealing temperature of 80 °C, deep donors with E_C – 0.16 eV are annealed in the irradiated crystals [8]. During annealing, shallow acceptors ionized at T = 78 K are formed, which leads to a decrease in the crystal resistance and a change in its conductivity type. After annealing at 130 °C, the

irradiated crystals were converted from *n* to *p*-type conductivity, as before irradiation. Neutron-irradiated crystals annealed at a temperature of 200 °C practically did not differ in electrical and optical properties from unirradiated CdSb crystals.

Problem setting. The aim of the paper is to consider methods for studying the kinetics and establishing the mechanisms of annealing of radiation defects in cadmium antimonide crystals.

Presentation of the main material. The processes of formation and rearrangement of radiation defects during irradiation and annealing can be considered as a set of quasichemical reactions of different orders. Some of them are difficult to reduce to a form that would allow analyzing the time dependence of the defect concentration during annealing.

Very often, the elementary activation annealing process is described by the equation:

$$\frac{dN}{d\tau} = -k_0 \cdot f(N) \cdot \exp\left(-\frac{E}{kT}\right), \tag{1}$$

where $\frac{dN}{d\tau}$ is the rate of change of the defect concentration at a constant annealing temperature and a constant activation energy of the process E;

N is the concentration of point defects or a physical parameter proportional to the concentration;

$f(N) = N^{\gamma}$ is some function;

γ determines the order of the process;

k_0 is a constant, which at $\gamma = 1$ is a frequency factor.

The simplest annealing of defects is the case where $\gamma = 1$ (a first-order process). Such a process occurs, for example, during the diffusion of defects (during annealing) to constant drains far from saturation. Most experimental data indicate that isothermal annealing curves described by first-order kinetics can be represented by an exponential function:

$$\frac{dN}{d\tau} = -kN, \tag{2}$$

where

$$k = AD, \tag{3}$$

N is the concentration of defects at time τ;

A depends on the geometry of the drains;

D is the diffusion coefficient.

The solution to Eq. 2 is:

$$N = N_0 \cdot \exp(-k\tau),$$

where N_0 is the concentration of defects at the initial moment of annealing, when $\tau = 0$.

The coefficient A in Eq. 3 can be determined knowing the geometry of the sinks. In the case when the sink is the outer surface of the crystal, the coefficient $A = \frac{\pi^2}{R^2}$ for a spherical surface with radius R and $A = \frac{\pi^2}{\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}}$ for a surface in the form of a rectangular parallelepiped with edge sizes a, b, c.

An important parameter that determines the kinetics of defect annealing is the annealing activation energy E. There are many methods for determining this energy. We used the cross-section method, which is based on the analysis of Arrhenius curves at different annealing temperatures.

The rate of change of the defect concentration at a constant annealing temperature and a constant activation energy is expressed by Eq. 1, written as:

$$\frac{1}{k_0} \cdot \frac{dN}{f(N)} = -\exp\left(-\frac{E}{kT}\right) d\tau. \tag{4}$$

Let us determine the change in the left-hand side of Eq. 4 for a certain time interval τ from the beginning of isothermal annealing:

$$-\frac{1}{k_0}\int_{N_0}^{N}\frac{dN}{f(N)}=\tau\cdot\exp\left(-\frac{E}{kT}\right), \tag{5}$$

where N_0 is the initial concentration of defects at time $\tau = 0$ (the beginning of annealing).

We will perform isothermal annealing at various close temperatures. At each temperature, we will choose such a time interval τ_0, during which the change in the defect concentration will be the same. Under such conditions, the left-hand sides of Eq. 5 will be the same, which we will denote by:

$$C=-\frac{1}{k_0}\int_{N_0}^{N}\frac{dN}{f(N)}. \tag{6}$$

Eq. 5, taking into account Eq. 6, will take the form:

$$\tau_0=C\cdot\exp\left(\frac{E}{kT}\right). \tag{7}$$

This Eq. 7 expresses the functional dependence between the annealing temperature T and the annealing time τ_0, during which the defect concentration decreases by the same amount at each annealing temperature. Taking the logarithm of Eq. 7, we obtain:

$$\ln\tau_0=\ln C+\frac{E}{kT}. \tag{8}$$

From the dependence $\ln\tau_0=f\left(\frac{1}{T}\right)$, we can determine the activation energy E of the process.

To determine the thermal stability region of radiation defects, the isochronal annealing method was used. The irradiated crystal was isothermally annealed for the same time interval $\Delta\tau=\tau_n-\tau_{n-1}$ at different temperatures T_1, T_2, T_3, ..., which increased after each previous annealing. The isochronal annealing curve can be obtained by integrating Eq. 1 over time:

$$\int_{N_n}^{N_{n-1}}\frac{dN}{N^{\gamma}}=k_0\cdot\exp\left(-\frac{E}{kT_n}\right)\Delta\tau. \tag{9}$$

Figure 1 shows the dependences of the time during which the resistance of the freshly treated surface decreased by a factor of e = 2.7 (in the exponential interval) on the storage temperature of the irradiated crystal. The activation energy of the process determined from this dependence using Eq. 8 is equal to (0.36 ± 0.03) eV. Obviously, this energy is the energy of defect migration, which is formed during the decay of defect clusters in neutron-irradiated CdSb crystals. For the exponential interval of the dependence of the resistance on time, we can determine the value k and, accordingly, the coefficient of defect diffusion D at different temperatures (Eq. 3).

When determining the coefficient A, it was assumed that the sink for defects is the surface of the crystal in the form of a parallelepiped, far from saturation. The calculated value of D at different temperatures is given in Table 1.

Table 1.

Temperature dependence of the diffusion coefficient D

T, K	D, cm^2/s
273	$1.6\cdot10^{-4}$
293	$3.6\cdot10^{-4}$
308	$7.6\cdot10^{-4}$
318	$1.4\cdot10^{-3}$

Conclusions. At annealing temperatures T_n, for which $kT_n << E$, the left-hand side of Eq. 9, which determines the change in the defect concentration during the annealing time $\Delta\tau$, will be very small. Significant annealing of defects will be observed at temperatures for which kT_n is close to the activation energy of defect annealing E. By conducting isochronal annealing, the main stages of annealing of radiation defects in irradiated crystals are established.

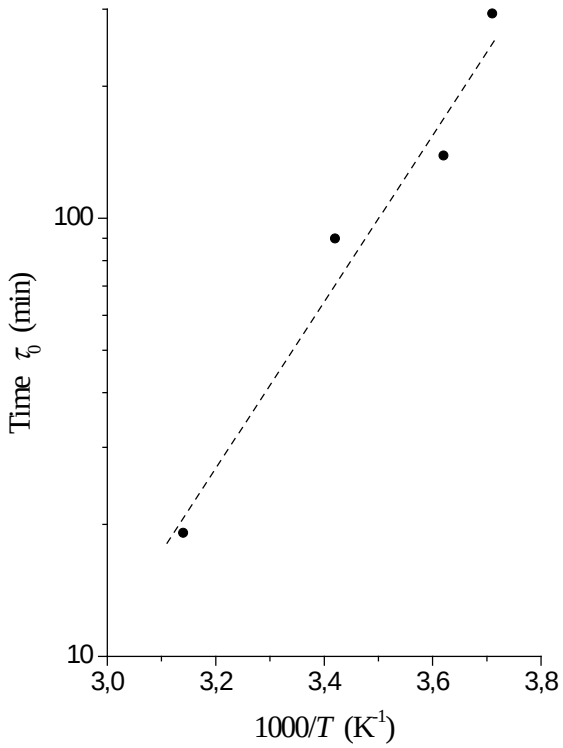

Fig. 1. **Temperature dependence of the time interval during which the defect concentration in the exponential region of the curves decreases by the same amount during annealing of neutron-irradiated ($\Phi = 2 \cdot 10^{18}$ n/cm^2) CdSb crystals**

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