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## **SOME FEATURES OF MODELLING DIFFUSIVE PROCESSES OF RELAXED OPTICS**

*Some problems of modelling the diffusive processes in Relaxed Optics are discussed. Diffusion processes in Relaxed Optics can occur at different stages. We will focus on processes that are caused by the absorption of optical radiation with an intensity slightly greater than the value required for the generation of maximum photokinetic defect in the near-surface region of the irradiated material, and less than the intensity required for the destruction of the irradiated material. The simulation was performed for antimonide and indium arsenide irradiated with 20 nanosecond pulses of a ruby laser. The model was based on a photoionization model: the generation of donor centers occurs due to the direct photoionization of two of the three chemical bonds of the two-dimensional sphalerite lattice. The rupture of the third bond leads to the generation of diffusion processes. Two diffusion models are presented. The one-diffusion model is based on the behavior and evolution of laser-induced donor centers as separate objects. The disadvantage of this model is that it cannot explain the tails of the donor center distribution profiles in the diffusion approximation. In this regard, a two-diffusion model was proposed, which is based on the idea of non-uniform photostimulated diffusion of atoms of the components of the irradiated material: indium and antimony for indium antimonide and indium and arsenic for indium arsenide. This is confirmed by experimental results for laser-irradiated cadmium telluride. The two-diffusion model allows us to explain the diffusion profiles of the distribution of donor centers in indium antimonide and indium arsenide in a consistent manner. Based on this model, it is concluded that such modeling methods can be extended to all binary compounds and it is worth expanding these methods to more complex materials (ternary, quaternary, etc.).*

**Key words:** diffusion, modelling, Relaxed Optics, indium antimonide, indium arsenide, cadmium telluride.

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## ДЕЯКІ ОСОБЛИВОСТІ МОДЕЛЮВАННЯ ДИФУЗІЙНИХ ПРОЦЕСІВ РЕЛАКСАЦІЙНОЇ ОПТИКИ

Обговорюються деякі проблеми моделювання дифузійних процесів релаксаційної оптики. Ці процеси в релаксаційній оптиці можуть відбуватися на різних стадіях процесу взаємодії лазерного випромінювання з речовою. Ми зосередимося на процесах, що спричинені поглинанням оптичного випромінювання з інтенсивністю, дещо більшою за значення, що необхідне для формування максимального фотокінетичного дефектоутворення в приповерхневій області опроміненого матеріалу, та меншою за інтенсивність, що необхідна для руйнування опроміненого матеріалу. Моделювання проводилося для профілів розподілу донорних центрів антимоніду індію та арсеніду індію, опромінених 20 наносекундними імпульсами рубінового лазера, отриманих методом вимірювання ефекту Холла з пошаровим стравлюванням. Модель базувалася на моделі фотоіонізації: генерація лазерно-індукованих донорних центрів відбувається внаслідок прямої фотоіонізації двох з трьох хімічних зв'язків двовимірної решітки сфалериту. Розрив третього зв'язку призводить до генерації дифузійних процесів. Наведено дві дифузійні моделі. Однодифузійна базується на поведінці та еволюції лазерно-індукованих донорних центрів як окремих фізичних величин. Недоліком цієї моделі є те, що вона не може пояснити хвости профілів розподілу донорних центрів в дифузійному наближенні. У зв'язку з цим була запропонована дводифузійна модель, яка базується на ідеї неоднорідної фотостимульованої дифузії атомів компонентів опроміненого матеріалу: індію та сурми для антимоніду індію та індію та міш'яку для арсеніду індію. Це підтверджується експериментальними результатами для опроміненого лазером телуриду кадмію отриманих за допомогою методу раманівського розсіяння. Дводифузійна модель дозволяє більш послідовно пояснити форму профілів розподілу донорних центрів в антимоніді індію та арсеніді індію в дифузійному наближенні. На основі цієї моделі зроблено висновок, що такі методи моделювання можна поширити на всі подвійні сполуки та варто розширити ці методи на більш складні матерали (потрійні, почетверенні та т.н.).

**Ключові слова:** дифузія, моделювання, релаксаційна оптика, антимонід індію, арсенід індію, телурид кадмію.

**Introduction.** Some problems of modelling the diffusive processes in Relaxed Optics are discussing. Diffusion processes in Relaxed Optics can occur at different stages.

We will focus on processes that are causing by the absorption of optical radiation with an intensity slightly greater than the value required for the generation of maximum photokinetic defect in the near-surface region of the irradiated material, and less than the intensity required for the destruction of the irradiated material (Heijmans, 2005). The simulation was performed for indium antimonide and indium arsenide irradiated with 20 nanosecond pulses of a Ruby laser (Trokhimchuk, 2016).

The model was based on a photoionization model: the generation of donor centers occurs due to the direct photoionization of two from the three chemical bonds of the two-dimensional sphalerite

lattice (Trokhimchuk, 2002; Trokhimchuk, 2016). Breaking the third bond leads to diffusion processes.

Two diffusion models are presented. The one-diffusion model is based on the behavior and evolution of laser-induced donor centers as separate objects. The disadvantage of this model is that it cannot explain the tails of the donor center distribution profiles in the diffusion approximation (Trokhimchuk, 2016).

In this regard, a two-diffusion model was proposed, which is based on the idea of non-uniform photostimulated diffusion of atoms of the components of the irradiated material: indium and antimony for indium antimonide and indium and arsenic for indium arsenide. This is confirmed by experimental results for laser-irradiated cadmium telluride (Prinsloo, 2003 – 2005). The two-diffusion model allows us to explain the diffusion profiles

of the distribution of donor centers in indium antimonide and indium arsenide in a consistent manner.

Based on this model, it is concluded that such modeling methods can be extended to all binary compounds and it is worth expanding these methods to more complex materials (ternary, quaternary, etc.) (Manning, 1968; Belova, 2017; Ganguly, 2002).

**Main results and discussions.** For illustration this method for Relaxed Optics we represent the simple model. The basic processes in this model are photostimulated and thermal (Trokhimchuk, 2016). The light source is monochromatic (laser). In this case we have one primary mechanism of optical scattering. Further, all possible primary processes of the interaction light with solid we were named scattering. For small intensity of the irradiation we have photostimulated processes basically, for large intensity – thermochemical and for the middle intensity we have both processes. Photostimulated processes may be cause of the creation of underthreshold defects for regular crystals and may be cause of annealing defects for irregular matter. Thermal processes are cause of finite distribution defects and ions including admixtures.

In general, the system of the equations for these processes is next. First equation is transfer (diffusion) equation (one-dimensional case) (Trokhimchuk, 2016)

$$\frac{\partial N}{\partial t} + a(x, t) \frac{\partial N}{\partial x} - D(x, t) \frac{\partial^2 N}{\partial x^2} = A e^{-\alpha x}, \quad (1)$$

Where

$$A = \frac{\alpha \eta (1-R) I_0}{h v \tau_r}, \quad (2)$$

Where  $N$  – concentration of the photostimulated damages (irreversible excitation of solid);  $\eta$  – coefficient of the creation the defect;  $R$  – the coefficient of optical reflection;  $x, t$  – space and time parameters respectively;  $I_0$  – the density of light flow;  $\tau_r$  – relaxation time;  $\alpha$  – light absorption index;  $h v$  – photon energy.

Time and boundary conditions have next forms:

$$N(x, 0) = N(\infty, t), \quad (3)$$

$$\left. \frac{\partial N}{\partial x} \right|_{x=0} = v N \Big|_{x=0}, \quad (4)$$

$$N(0, \tau_i) = A. \quad (5)$$

The conditions (3) are evident. Condition (4) is illustrated the motion of excitations in crystal volume because one (defects) are annealed on surface. Condition (5) has place for case when processes optical generation of defects is more intensive than thermal relaxed processes.

Second equation (heat conductivity) for one-dimensional case may be written in the next form

$$\frac{\partial^2 T}{\partial x^2} - \frac{1}{\kappa} \frac{\partial T}{\partial t} = \frac{\alpha(1-R)I_0}{k\tau_i} \exp(-\alpha x) \quad (6)$$

with time and border conditions

$$T(x, 0) = 0, \quad (7)$$

$$T(\infty, t) = 0, \quad (8)$$

where  $T$  – temperature;  $\kappa, k$  – coefficients of temperature and heat conductivity, respectively.

Solution system (6)–(8) has next kind for volume semiconductor

$$T(x, t) = \frac{\alpha(1-R)I_0}{k\tau_i} (\kappa t)^{1/2} i \operatorname{erfc} \left[ \frac{x}{\alpha(\kappa t)^{1/2}} \right] \quad (9)$$

and for surface

$$T(0, t) = \frac{\alpha(1-R)I_0}{k\tau_i} \left( \frac{\kappa t}{\pi} \right)^{1/2}. \quad (10)$$

With help solutions (9), (10) we can receive the temperature dependence for main phenomenological coefficients of system (1)–(5).

For explanation basic experimental data about interaction ruby laser radiation with InSb and InAS the system (1) – (5) may be represented in more simple form (Trokhimchuk, 2016)

$$\frac{N}{\tau'} - D \frac{\partial^2 N}{\partial x^2} = \frac{\alpha \eta (1-R) I_0}{h v \tau_r} e^{-\alpha x}, \quad (11)$$

with time and border conditions (3) and (4).

For case  $L \gg x$ , where  $L$  is diffusion length, solution of (11) has next form

$$N = \frac{\alpha \eta \tau' (1-R) I_0}{(\alpha^2 L^2 - 1) \tau_r} \left[ \frac{\alpha L^2 + v \tau_r}{L + v \tau_r} \exp\left(-\frac{x}{L}\right) - \exp(-\alpha x) \right]. \quad (12)$$

Further, we can neglect the surface phenomena ( $\alpha L^2, L \gg v \tau_r$ ). It correspond the experimental data the irreversible interaction in volume (but not surface) semiconductor. In this case (12) has next form

$$N = \frac{\alpha \eta \tau' (1-R) I_0}{(\alpha^2 L^2 - 1) \tau_r} \left[ \alpha L \exp\left(-\frac{x}{L}\right) - \exp(-\alpha x) \right]. \quad (13)$$

For finding layer concentration (13) must be multiplied on  $x$ . Result of this is next

$$N = \frac{\alpha \eta \tau' (1-R) I_0 x}{(\alpha^2 L^2 - 1) \tau_r} \left[ \alpha L \exp\left(-\frac{x}{L}\right) - \exp(-\alpha x) \right]. \quad (14)$$

The relaxation time  $\tau_r$  is determined from functional dependence  $T(x, t)$  for each layer and corresponding diffusion coefficient is determined as

$$D = D_0 \exp\left(-\frac{E_a}{k_B T}\right). \quad (15)$$

Where  $k_B$  is Boltzmann constant.

From (14) we can receive two border approximations. First is named kinetic ( $\alpha L \ll 1$ )

$$N_{k_s} = \frac{\alpha \eta \tau' (1-R) I_0 x}{h v \tau_r} \exp(-\alpha x) \quad (16)$$

and second is named dynamic ( $\alpha L \gg 1$ )

$$N_{D_s} = \frac{\eta \tau' (1-R) I_0 x}{h v \tau_r} \exp\left(-\frac{x}{L}\right). \quad (17)$$

Now we go to one-diffusion approximation. With help of formulas (14), (16), (17) the calculated profiles of distribution of donor centers in InSb after ruby laser irradiation were received (Trokhimchuk, 2016).

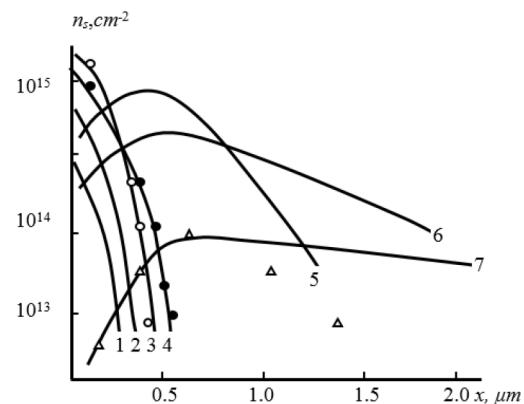
As the basis of calculation the next conditions and approximations were be used

$$L = D_{0\tau_r} \exp\left(-\frac{E_a}{k_B T}\right). \quad (18)$$

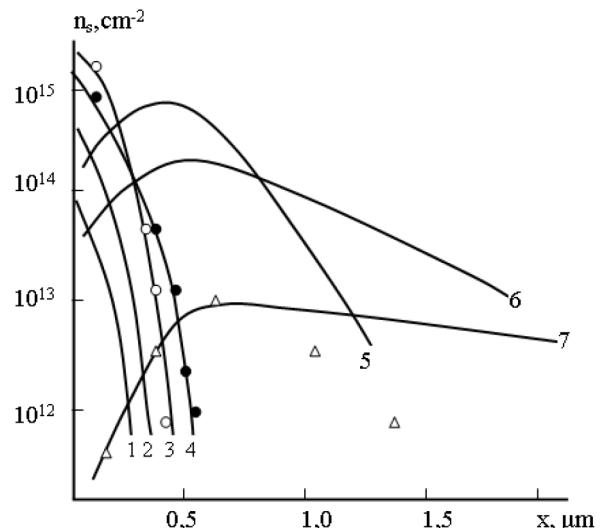
In this approximation we have one mechanism of the scattering as  $D_0 = 0.05 \text{ cm}^2 \cdot \text{s}^{-1}$  is coefficient of the self-diffusion atoms of In;  $E_a = 1.81 \text{ eV}$  is energy of the activity the self-diffusion atoms of In (Trokhimchuk, 2016);  $\tau_r$  is determined with functional dependence  $T(t)$  and equal  $(10 \div 10^3) \tau_i$ ;  $\tau' \sim 10^{-7} \text{ s}$  – the time of the life the unstable carriers in crystal (Trokhimchuk, 2016);  $R = 0.45$  for  $h v = 1.78 \text{ eV}$ ;  $\eta = 0.2$  (ionic mechanism);  $\alpha = 2 \cdot 10^5 \text{ cm}^{-1}$ ;  $t_i = 2 \cdot 10^{-8} \text{ s}$ . The binding calculated results to experimental data were provided for  $I_0 = 0.1 J \cdot \text{cm}^{-2}$ .

In Fig.1, the main calculated data coincide with experimental results. More high value the theoretical data for curve 7 is explained the dependence of diffusion coefficient from depth.

Analogous results were received for InAs. Modeling profiles of distribution of laser-generated donor centers are represented in Fig. 2 (Trokhimchuk, 2016).



**Fig. 1. Calculated profiles of the distribution the concentration of donor centers in InSb for various conditions of irradiation**  
 $(J \times \text{cm}^{-2}; \text{curve 1} - 0.018; 2 - 0.04; 3 - 0.07;$   
 $4 - 0.096; 5 - 0.12; 6 - 0.14; 7 - 0.16)$   
 (Trokhimchuk, 2002)



**Fig. 2. Calculated profiles of the distribution the concentration of donor centers in InAs for various regimens of irradiation**  
 $(J \times \text{cm}^{-2}; \text{curve 1} - 0.04; 2 - 0.07; 3 - 0.12;$   
 $4 - 0.16; 5 - 0.20; 6 - 0.25; 7 - 0.3)$   
 (Trokhimchuk, 2016)

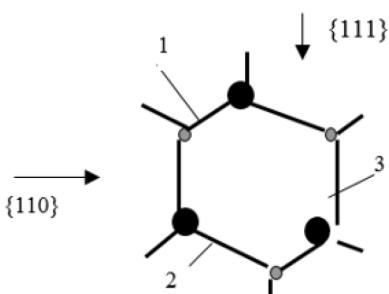
The rough estimation of the effective section of the scattering may be represented as the next schema. The absorption index  $\alpha$  of the light has next kind (3.38).

$$\alpha = \sum_i N_i \sigma_i, i \in (In, Sb), \quad (19)$$

where  $N_i$  is the concentration of proper centers of light scattering,  $\sigma_i$  is scattering cross-section of proper centers.

For self-absorption the number of the scattering centers  $N_i$  is equal the atom density the lattice.

For InSb  $N \sim 4 \times 10^{21} \text{ cm}^{-3}$ ; for ruby laser  $\alpha = 2 \times 10^5 \text{ cm}^{-1}$ . For this case the section of effective scattering (absorption)  $\sigma = \alpha/N = 5 \cdot 10^{-17} \text{ cm}^{-2}$ . For more detail estimation, the effect of the anisotropy the absorption the laser irradiation we are used the two-dimensional lattice (Fig.3) (Trokhimchuk, 2016).



**Fig. 3. Two-dimensional picture the crystal lattice  $A_3B_5$  (including InSb and InAs) the cubic symmetry (sphalerite). Bond 1 is pure covalent. Bond 1 is corresponded to band gap and has value 0,18 eV, bond 2 – 1,95 eV and bond 3 – 2,15 eV. For InAs bond 1 has value 0,36 eV, bond 2 – 3,8 eV and bond 3 – 4,2 eV (Trokhimchuk, 2016)**

The bond 1 is corresponded the pure covalent bond: for InSb and InAs one is equal the sum of the corresponding covalent radii. For InSb the length of the bond 1 is equal  $2.8 \times 10^{-8} \text{ cm}$ . The angle between directions  $\{111\}$  the bond 1 and  $\{110\}$  is equal  $37,5^\circ$  for the bond 1. The meaning the “length of the scattering” for our estimation is  $7 \times 10^{-9} \text{ cm}$ . The “effective length” the covalent bond for directions  $\{110\}$  and  $\{111\}$  is equal  $1,56 \times 10^{-8} \text{ cm}$  and  $2,33 \times 10^{-8} \text{ cm}$  respectively. For spherical, elliptical and dumbbells configurations the effective section of the scattering is meant from  $(4–6) \times 10^{-17} \text{ cm}^{-2}$ . The more small meaning the section of the scattering than square of the “effective length” is explained the large volume the “ionic centers” of In and Sb. For this estimation coefficient of the anisotropy the absorption, including the surface density of covalent bonds, is equal the square of the tangent of our angle – 0,45. The experimental data (Trokhimchuk, 2016) is corresponded our estimation.

For more precisions modeling of results, which are represented on Fig. 2.5, will consider now, as a difference of coefficients of self-diffusion of indium and antimony influences on forming of profiles of distribution of donor centers in indium antimonite under irradiation of pulses of Ruby laser by pulse duration of 20 ns.

For one coefficient of diffusion, the general view of the formula for the profile of distribution of donor centers has form (14) (Trokhimchuk, 2016).

Further we used kinetic (formula (16)) and dynamic (formula (17)) approximations. Diffusion length is determined by means of correlation:

$$L = \sqrt{D\tau_r}. \quad (20)$$

It should be noted that the profiles of distribution are necessary to be calculated using a formula (14). However, at the calculation of the left part of the curves of Fig. 1 (subsurface region), it is possible to use correlation (16), and at the calculation of right part of curves is correlation (17).

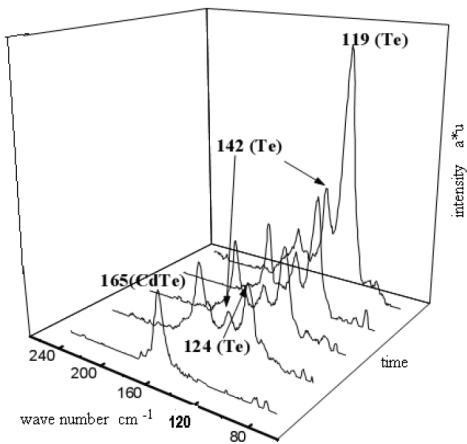
For more precisions modelling, we must go from the one-diffusive approximation to two-diffusive approximation and use these results for the modelling for InSb and InAs. Instead of diffusion of donor centers will examine self-diffusion of atoms of indium and antimony, which are caused by the secondary effects of Relaxed Optics. As known from literature (Trokhimchuk, 2016) the atoms of indium and antimony or indium and arsenic have different coefficients of self-diffusion. In addition, according to the Kapayev–Kopayev–Molotkov theory (Trokhimchuk, 2016) the intensive generation of electrons (in our case of donor centers) realizes in a subsurface layer, that is why it follows to expect that a subsurface area is anymore enriched by the ions of antimony. The coefficient of self-diffusion (more correct it will be to say the photostimulated diffusion) of atoms of antimony less than of atoms of indium. It is confirmed to the experimental results of L. Prinsloo and M. Lee (Prinsloo, 2003–2005) for the actions of radiation of argon laser on to the cadmium telluride: the ions of tellurium remain in a subsurface area, while the ions of cadmium go to the depth of the irradiated material.

Tendency of the creation of tellurium on surface CdTe after argon-laser irradiation (wavelength 514.5 nm) under intensity of irradiation was observed in (Prinsloo, 2003–2005). Irradiation in the region of destruction of surface was carried in continuous regime with duration of irradiation 60 s. Power of irradiation was oscillated from 1 mW to 10 mW, diameter of irradiated surface – from 2  $\mu\text{m}$  to 12  $\mu\text{m}$ . Band gap of CdTe (thermal dependence) is equaled

$$E_g = (1.605 - 4.9 \cdot 10^{-4}T) \text{ eV},$$

where  $1.605 \text{ eV}$  – band gap of CdTe under temperature  $2\text{K}$ . Photon energy of laser irradiation  $h\nu = 2.41 \text{ eV}$ . Another words we have case  $h\nu > E_g$ .

Typical spectra of Raman scattering for CdTe and Te are represented in Fig. 4.



**Fig. 4. Spectra of Raman scattering under irradiation with  $w < 3 \text{ kW} \cdot \text{cm}^{-2}$  (Prinsloo, 2003–2005)**

Furthermore, if for silicon we must proof various mobility of atoms – partners of covalent bonds, for cadmium telluride, this question is resolved because atoms of Te and Cd have various mobility's (various self-diffusive coefficients). An appearance of Te peaks may be caused or migration atoms of Cd in volume of irradiated materials or it particular sublimation. Considering that value of intensity of irradiation has place near threshold of destruction of semiconductors, sublimation of cadmium is process that is more possible because cadmium as metal has more large mobility as tellurium).

As can be seen from represented data we can't speak about annealing of damages in irradiated cadmium telluride. Nature of these phenomena is next: stratification of semiconductor is realized and new stable states and phases may be generated. An appearance of separate regions of atoms tellurium and cadmium on surface (Prinsloo, 2003 – 2005) is caused of diffractive structure of focused laser beam. In the region of diffractive maximums sublimation of cadmium is basic process and therefore rest layers are enriched of atoms of tellurium; in the region of diffractive minimums – “superstructural” subsurface layers of cadmium. Sublimation and diffusion in volume of materials of atoms of cadmium are realized for irradiation for less intensity of irradiation too, therefore peaks

of tellurium are presented in Raman spectra for all represented diapason of irradiation (Fig. 4).

Literary data for self-diffusion of atoms of indium and furnace in the indium antimonite are contradictory (Trokhimchuk, 2016). Therefore will use those data that correspond to experimental data, namely, the coefficient of self-diffusion of atoms of indium is higher, than of antimony.

For the estimation of diffusive «tails» of curves 5–7 of Fig. 2.5, we are using modified formula (17) for the ions of antimony and indium

$$N_{D_{si}} = \frac{\eta\tau'(1-R)I_0x}{h\nu\tau_r} \exp\left(-\frac{x}{L_i}\right), \quad i \in (In, Sb). \quad (17a)$$

Concordantly (Shaw, 1973) temperature dependence of coefficients of diffusion is represented in a kind

$$D = D_{0i} \exp\left(-\frac{Q_i}{k_B T}\right), \quad i \in (In, Sb), \quad (15a)$$

where  $Q$  – proper activation energy of self-diffusion.

For a calculation we select next data (Trokhimchuk, 2016)

$$D_{0Sb} = 3.1 \cdot 10^{13} \text{ cm}^2/\text{s}, \quad D_{0In} = 1.76 \cdot 10^2 \text{ cm}^2/\text{s}.$$

Farther a calculation was conducted thus. The descriptions resulted in got out for a calculation (Trokhimchuk, 2016), however correlation of energies of activating of self-diffusion undertook to such as in (Shaw, 1973), what correspond to experimental data. Then in obedience to formula (15) the coefficient of self-diffusion of antimony was estimated for the temperature of  $800\text{K}$  (temperature of melting of indium antimonide). In future, a scenario of calculation was following. Diffusive length of  $0.7 \mu\text{m}$  (a curve 7 Fig. 1) is corresponded to diffusion of antimony, as we get the inverted layer of donor type on substrate of p-type. Relaxation time is equalled of relaxation  $\tau_r = 10^3\tau_i = 2 \cdot 10^{-5} \text{ s}$ . Then, the coefficient of diffusion of atoms of antimony is determined from equation:

$$D_{Sb} = \frac{L_{Sb}^2}{\tau_r} = 2.45 \cdot 10^{-4} \text{ cm}^2/\text{s}.$$

The obtained calculation data allow quality to explain behaviour of «tails» of curves of Fig. 1. Depth of formation of donor centers for a curve 7 of Fig. 1 ( $\sim 1.5 \mu\text{m}$ ) approximately corresponded a depth on that the concentration of centers of p-type

(atoms of indium) becomes more than concentration of centers of n-type (atoms of antimony). From the value of this length, which is calculated according

to correlation  $x_{eq} = \frac{L_{In}L_{Sb}}{L_{In} - L_{Sb}} \ln \frac{L_{In}}{L_{Sb}} = 1.5 \mu m$ , we get diffusive run-length of atoms of indium  $L_{In} = 4.2 \mu m$ .

The coefficient of diffusion of atoms of indium is determined like analogous to as a antimony and equal

$$D_{In} = \frac{L_{In}^2}{\tau_r} = 8.82 \cdot 10^{-3} \text{ cm}^2/\text{s}.$$

Having these data, we can now define energies of activation of the photostimulated diffusion of atoms of indium and antimony. They are determined from equation

$$Q_{In(Sb)} = kT \ln \frac{D_{0In(Sb)}}{D_{In(Sb)}}.$$

After substitution of corresponding data we have  $Q_{In} = 2.45 \text{ eV}$ ,  $Q_{Sb} = 2.71 \text{ eV}$ . Literary data (Atomic, 1973) give value  $Q_{In} = Q_{Sb} = 4.3 \text{ eV}$ . These data behave to material of n-type. We have an irradiation of material of p-type, and for this material the atoms of indium have more mobility than atoms of antimony. Naturally, we must take into account and diffusion (radiation (photo) stimulated (Trokhimchuk, 2002)) that decreases energy of activation.

These calculations allow quality correctly to explain the tendency of behaviour of tails of profiles of distribution of «diffusive» type (curves 5–7 of Fig. 1) of donor photostimulated centers, in the indium antimonite, and in principle, this method of calculation can be extended on all double compounds, including the processes of the laser alloying of cadmium telluride with a help of the radiations of argon laser (Prinsloo, 2003 – 2005).

Analogous results were receiving for indium arsenide (Trokhimchuk, 2016). Data for estimation was next  $D_{0In} = 6 \cdot 10^5 \text{ cm}^2/\text{s}$ ,  $D_{0As} = 3 \cdot 10^7 \text{ cm}^2/\text{s}$ , relaxation time  $\tau_r = 10^3 \tau_i = 2 \cdot 10^{-5} \text{ s}$ . Diffusion length of As atoms is equal  $0.7 \mu m$  (for curver 7 of Fig. 2). From the value of this length, which is calculated according to correlation

$x_{eq} = \frac{L_{In}L_{As}}{L_{In} - L_{As}} \ln \frac{L_{In}}{L_{As}} = 1.5 \mu m$ , we get diffusive run-length of atoms of indium  $L_{In} = 4.2 \mu m$ . Proper coefficients of self-diffusion are equaled  $D_{As} = \frac{L_{As}^2}{\tau_r} = 8 \cdot 10^{-4} \text{ cm}^2/\text{s}$ ,  $D_{In} = \frac{L_{In}^2}{\tau_r} = 3 \cdot 10^2 \text{ cm}^2/\text{s}$  and energy of diffusion activation –  $Q_{In} = 1.76 \text{ eV}$ ,  $Q_{As} = 2.8 \text{ eV}$ .

The represented two-diffusive model over shows as far as effective there can be an account of different mobility of atoms-components of semiconductor (in this case indium antimonite) for explanation of effects of irreversible interaction of laser radiation with semiconductors.

For more detailed description, design and explanation of effects of irreversible interaction of laser radiation with semiconductors it is necessary to develop the methods of nonlinear dynamics.

Based on this model, it is concluded that such modeling methods can be extended to all binary compounds and it is worth expanding these methods to more complex materials (ternary, quaternary, etc.). This is necessary in order to adequately explain and describe the relevant experimental results for the  $Hg_xCd_{1-x}Te$  (Bahir, 1981). In this case, we can use the concept of the Manning factor (Manning, 1968), which is successfully used to describe diffusion processes in complex systems (Belova, 2017; Ganguly, 2002; Haitjanas, 2005).

### Conclusions.

1. Some problems of modelling diffusive processes of Relaxed Optics for indium antimonite and indium arsenide are discussed.

2. The system of photokinetic and heat-conductivity equations were selected for modelling.

3. Particular case of general resolution of this system equations (dynamic approximation) was used for the modelling the diffusion processes.

4. One-diffusion approximation allow explaining left parts of diffusion profiles of distribution of laser-induced donor centers.

5. Two diffusive approximation allow explaining the behavior of all diffusion profiles.

6. It is advisable to expand and adapt these modeling methods for more complex compounds (ternary, quaternary, etc.)

### BIBLIOGRAPHY:

1. Bahir G., Bernstein T. cw CO<sub>2</sub> and ruby laser annealing of ion-implanted Hg<sub>x</sub>Cd<sub>1-x</sub>Te. *Applied Physics Letters*, v.39, No.9, 1981. P.730–732.
2. Belova I. V., Ahmed T., Sarder U., Evteev A. V., Levchenko E. V., Murch G. E. The Manning factor for direct exchange and ring diffusion mechanisms. *Philosophical Magazine*, vol. 97, is. 4, 2017. P. 230–247.
3. Boltaks B. I. Diffusion in Semiconductors. London, Melbourne: Hassell Street Press, 2021. 400 p.
4. Ganguly J. Diffusion kinetics in minerals: Principles and applications to tectono-metamorphic processes. *EMU Notes in Mineralogy*, Vol. 4, Chapter 10, 2002. P. 271–309.
5. Heitjans P., Kärger J., eds. Diffusion in condensed matter: Methods, Materials, Models (2nd ed.). Berlin – Heidelberg, 2005. 965 p.
6. Manning J. Diffusion Kinetics for Atoms in Crystals. Princeton: Van Nostrand, 1968. 275 p.
7. Prinsloo L.C., Lee M. E. Laser induced formation of a Te on CdTe. Internet Archive (University of Pretoria @ University of North, South Africa) 2003–2005. 2 p.
8. Shaw D., eds. Atomic diffusion in semiconductors. Ed. by New York: Plenum Press, 1973. XIII+607 p.
9. Trokhimchuk P. P. Relaxed optical phenomena in InSb and InAs and comparative analysis with other experimental data./Proc. SPIE/Ukraine. *Current Research in Optics and Photonics*. № 2, 2002. P. 110–118.
10. Trokhimchuk P. P. Relaxed Optics: Realities and Perspectives. Saarbrücken: Lambert Academic Publishing, 2016. 260 p.

### REFERENCES:

1. Bahir, G., & Bernstein, T. (1981) *cw CO<sub>2</sub> and ruby laser annealing of ion-implanted Hg<sub>x</sub>Cd<sub>1-x</sub>Te*. *Applied Physics Letters*, v.39, No.9, pp.730–732.
2. Belova, I. V., Ahmed, T., Sarder, U., Evteev, A. V., Levchenko, E. V., & Murch G. E. (2017) *The Manning factor for direct exchange and ring diffusion mechanisms*. *Philosophical Magazine*, vol. 97, is. 4, pp. 230–247.
3. Boltaks, B. I. (2021) Diffusion in Semiconductors. London, Melbourne: Hassell Street Press, 400 p.
4. Ganguly, J. *Diffusion kinetics in minerals: Principles and applications to tectono-metamorphic processes*. EMU Notes in Mineralogy, Vol. 4, Chapter 10, 2002. P. 271–309.
5. Heitjans, P., Kärger, J., eds. (2005) Diffusion in condensed matter: Methods, Materials, Models (2nd ed.). Berlin – Heidelberg, 965 p.
6. Manning, J. *Diffusion Kinetics for Atoms in Crystals* (1968). Princeton: Van Nostrand, 275 p.
7. Prinsloo, L. C., & Lee M. E. (2003–2005) Laser induced formation of a Te on CdTe. Internet Archive (University of Pretoria @ University of North, South Africa). 2 p.
8. Shaw, D. (1973) eds. Atomic diffusion in semiconductors. Ed. by D. Shaw. New York: Plenum Press, XIII+607 p.
9. Trokhimchuk, P. P. (2002) *Relaxed optical phenomena in InSb and InAs and comparative analysis with other experimental data*. Proc. SPIE/Ukraine. *Current Research in Optics and Photonics*, № 2, pp.110–118.
10. Trokhimchuk, P. P. (2016) Relaxed Optics: Realities and Perspectives. Saarbrücken: Lambert Academic Publishing, 260 p.

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