ON THE MODEL OF RADIATION-INDUCED ORDERING OF THE DEFECT STRUCTURE IN CdS CRYSTALS

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A physical and mathematical model of the radiation-induced ordering of the defect structure in CdS crystals is proposed. The key points of the model are the gettering of defects (Cd_i) at sinks with regard for a substantial (by about 2 orders of magnitude) increase of the diffusion coefficient of of defects under irradiation and the increase of the defect lifetime at irradiation doses below 750 R.

The action of ionizing radiation on semiconducting compounds and semiconductor-based structures is governed by at least two competitive processes: the generation of radiation-induced defects and the radiation-induced evolution of structural defects; the latter is accompanied by the improvement of the electrophysical characteristics of crystals and devices. The studies of the radiation action on electrical, optical, and structural properties of the A_3B_5-semiconductor-based barrier structures revealed the effect of radiation-induced improvement of their characteristics at small doses of electron and gamma-ray irradiation [1–4]. While analyzing the results made by the authors of those works, two basic explanations of the mechanism of this effect can be offered:

1) the reconstruction of the bulk recombination centers intensifies near the surface, because the interatomic bonds in the crystal become weakened here;

2) the semiconductor–metal interfaces, which are effective sinks, serve for gettering the recombination-active impurities or defects.

The character of a radiation-induced modification of the lifetime of minority current carriers depends substantially on the initial deficiency of the crystal and the recombination activity of its centers. If the irradiation intensity is at a subthreshold level, the rate of diffusion processes is higher for those atoms, the oscillations of which are thermalized for longer times and depend linearly on the irradiation intensity [5].

Earlier [6–9], we found that, as the irradiation dose D increases, the efficiency of radiation-induced modifications of the semiconducting structure parameters has a tendency to saturation, which also correlates with the data of works [1–4].

At the initial stage ($D \leq 10^3$ R) of X-ray irradiation of Au-CdS barrier structures, the improvement of the electrophysical parameters of their current-voltage characteristics and a reduction of the characteristic maximum, which appeared in their capacitor-voltage characteristics upon the formation of barrier structures, to a background level (Fig. 1) are observed. If the irradiation doses are $D > 10^3$ R, the generation and accumulation of radiation-induced defects in the CdS-based surface-barrier structures start to dominate over the "curing" of structural defects. Therefore, the electrophysical parameters of those structures become worse.

The researches of processes that take place at the initial stage of the irradiation of bulk CdS crystals were described in work [10]. In Fig. 2, the temperature dependences of the Hall mobility of current carriers in irradiated CdS crystals are shown. The analysis of these results allows us to assert that, provided the irradiation doses are lower than 750 R and the current carrier concentration is constant, the mobility of the latter, as well as the related conductivity of the specimen, grows

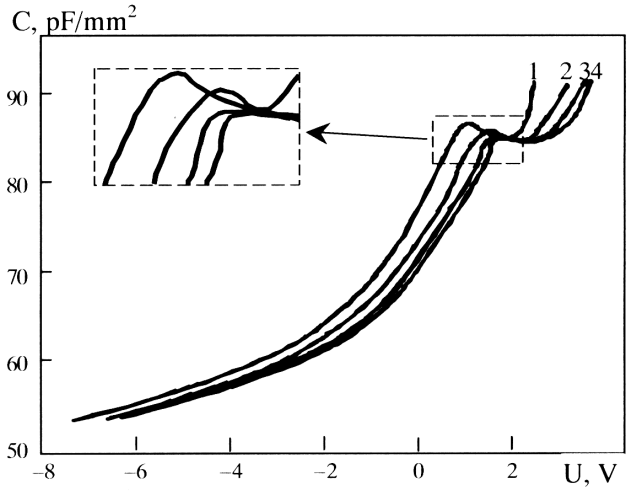

Fig. 1. High-frequency capacitor-voltage characteristics of Au-CdS-based diodes before (*1*) and after irradiation up to the dose 350 (*2*), 10^3 (*3*), and 3×10^4 R (*4*)

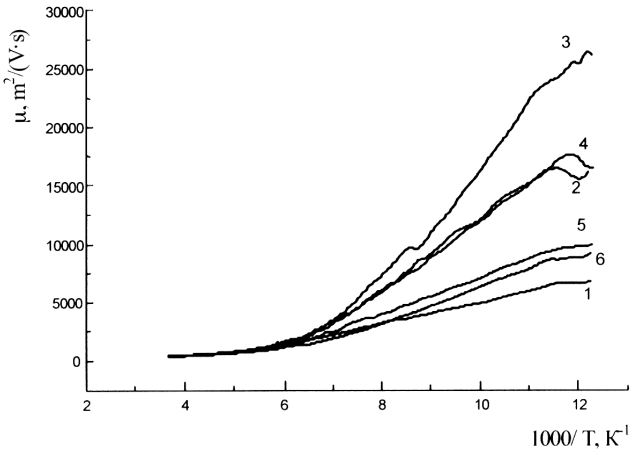

Fig. 2. Temperature dependences of the Hall mobility of current carriers in irradiated CdS crystals: (*1*) before irradiation, (*2*) at $D = 500$, (*3*) 750, (*4*) 1000, and (*5*) 1400 R, and (*6*) after the 96-h annealing of the specimen at room temperature

at a temperature fixed. A further increase of the irradiation dose leads to a reduction of the current carrier mobility and, correspondingly, to a diminishing of the crystal conductivity.

This work aimed at constructing the physical and mathematical model for the effect of radiation-induced ordering of the defect structure in CdS crystals, taking into account our experimental results and those found in the literature. In order to describe this effect, we used a modified equation of diffusion, which made allowance for a significant growth of the diffusion coefficient of the interstitial component undergone the action of radiation:

$$\frac{\partial N(x,t)}{\partial t} = G - \frac{N(x,t)}{\tau(t)} + D^* \frac{\partial^2 N(x,t)}{\partial x^2}, \qquad (1)$$

where $N(x,t)$ is the concentration distribution of interstitial cadmium (Cd_i), D^* the diffusion coefficient of Cd_i under ionizing radiation, G the generation rate of Cd_i, and $\tau(t)$ the Cd_i lifetime.

Assuming that the most effective sinks for Cd_i are dislocations and free surfaces, the boundary conditions can be written down in the form

$$N(0,t) = N_0 \exp(\alpha t),$$

$$N(a,t) = N_0 \exp(\beta t), \qquad (2)$$

where $N(0,t)$ and $N(a,t)$ are the Cd_i concentrations at the specimen edges, a is the specimen length, N_0 the average Cd_i concentration, and α and β are certain constants. The initial concentration profile $N(x,0)$ was taken in the form of the normal Gaussian distribution.

High diffusion coefficients of the components are known to predetermine a reduction of the near-surface gradient of the interstitial atom concentration. Concerning the effect which we analyze taking into account the boundary conditions, the value of the diffusion coefficient can also affect the level of the average Cd_i concentration in the crystal. Therefore, our model, which describes the effect of radiation-induced ordering, takes into account both the variation of the defect lifetimes and the growth of the diffusion coefficient in the radiation field.

Making use of the Crank—Nicolson method of finite differences [11] and having written down the corresponding recurrence equations with boundary conditions, we obtain the expression

$$\frac{N(x,t+k) - N(x,t)}{k} =$$

$$= D\Big[N(x-h,t+k) - 2N(x,t+k) + N(x+h,t) +$$

$$+ N(x-h,t) - 2N(x,t) + N(x+h,t)\Big]/[2h^2], \qquad (3)$$

where h and k are the mesh widths along the x- and t-variables, respectively.

While solving our problem (1), we may attempt to find a solution in the analytical form [11, 12]. In this case, taking $N(x,t)$ in the form $N(x,t) = X(x) + T(t)$, we obtain

$$N(x,t) = C_1 \sin\left(\frac{x}{\sqrt{D^*\tau}}\right) +$$

$$+ C_2 \cos\left(\frac{x}{\sqrt{D^*\tau}}\right) + G\tau + C_3 \exp\left(\frac{t}{\tau}\right), \qquad (4)$$

where C_{1-3} are constants. Taking into account the initial and boundary conditions (2) which were adapted for our method, we obtain

$$N(x,t) = f(x) + \left\{G\tau - \left[N_0 \exp(\alpha t) \sin\left(\frac{a-x}{\sqrt{D^*\tau}}\right) +\right.\right.$$

$$+ N_0 \exp(\beta t) \cos\left(\frac{x}{\sqrt{D^*\tau}}\right) - \Big[f(x) - G\tau \times$$

$$\times \left(1 - \exp\left(-\frac{t}{\tau}\right)\right)\Bigg] \sin\left(\frac{a}{\sqrt{D^*\tau}}\right)\Bigg] \Big/ \Bigg[\sin\left(\frac{a-x}{\sqrt{D^*\tau}}\right) +$$

$$+ \sin\left(\frac{x}{\sqrt{D^*\tau}}\right) - \sin\left(\frac{a}{\sqrt{D^*\tau}}\right) \exp\left(-\frac{t}{\tau}\right)\Bigg]\Bigg\} \times$$

$$\times \left(\exp\left(-\frac{t}{\tau}\right) - 1\right), \qquad (5)$$

where $f(x)$ is a function setting the initial distribution.

The experimental researches and the modeling of the diffusion of components in CdS crystals provided us with information concerning the dependences of the concentration of interstitial Cd atom defects $N(x,t)$ on the crystallographic orientation of the specimen, as well as the defect lifetimes before and after irradiation, and the variation of the diffusion coefficient. Those dependences allowed us to estimate the character of the concentration profile change in time, in particular to analyze the diffusion of interstitial cadmium (Cd_i) towards the free surfaces and the spatial variation of its concentration.

We note that all the results that were obtained using two programs (the analytical and numerical solutions of the problem concerned) turned out almost identical. The average mismatch between the corresponding output data amounted to no more than 1%. Therefore, we were able to use one of the programs, e.g. the analytical solution, to solve the direct problem, while the other to solve the inverse one, i.e. searching for the values of diffusion parameters provided the known concentrations.

The following values of the parameters were taken as initial ones while modeling the diffusion of defects in CdS crystals: the diffusion coefficients $D = 10^{-16}$ m^2/s under normal conditions and $D^* = 10^{-13}$ m^2/s under irradiation; the generation rate of defects in the semiconductor under irradiation $G = 10^{16}$ m$^{-3} \times$ s^{-1}; the average lifetime of a defect in the crystal without irradiation $\tau \approx 10^3$ s; the initial distribution $N(x,0)$ had the form of the normal Gaussian distribution $\left(\frac{1}{\sqrt{2\pi\sigma}} \exp\left[-\frac{(N(x,0)-N_0)^2}{2\sigma^2}\right]\right)$, where the average value of the defect concentration was $N_0 = 10^{21}$ m^{-3}; the specimen thickness $L = 7 \times 10^{-4}$ m; the coefficients in the boundary conditions $\alpha = \beta = 1.7 \times 10^{-3}$ s^{-1}; the duration of the experiment was from 1000 to 15000 s; the thickness of the near-surface layer and the excess concentration of defects in it were of about 10^{-6} cm and 10^{20} m^{-3}, respectively.

It is known [13] that the concentration of defects in the near-surface region of the basic facets of CdS crystals is substantially higher than that in the bulk. The consequence of such a distribution of defects (Cd_i) is a manifestation of the abnormal temperature dependence of the surface conductivity along the basic crystal facets (an increase of the conductivity by 3 to 4 orders of magnitude, if the specimens are cooled from room temperature down to 80 K), as well as the electron emission emergence from these facets, if the specimens are cooled down in the same temperature range [14]. The surface electron concentration in the formed low-resistance layer of a high-resistance CdS crystal ($\rho = 2500\ \Omega \times$ cm^{-1}), which was estimated from the residual conductivity of the specimen, was $N_s = 10^{12}$ cm^{-2}. The near-surface region, where the maximal concentration of interstitial Cd is localized, extends towards the crystal depth to $d \leq 2 \times 10^{-6}$ cm. While interpreting the results that were used for modeling the radiation-induced processes in the crystals and the surface-barrier structures, we assumed that there occurred a reconstruction of metastable defects, in which shallow donor centers (Cd_i) participated. In so doing, we accepted that the concentration profile of the defect distribution in the specimen was at equilibrium and did not change in time. The physical model of radiation-induced improvement of the parameters takes the following factors to be responsible for the variation rate of the concentration of defects:

— gettering of the defects at dislocations;

— recombination processes, whose efficiency depends on the temperature of the crystal [2];

— under the irradiation of CdS crystals, the diffusion coefficient of interstitial Cd increases by 2–3 orders of magnitude [5] (depending on specific conditions), and, on the other hand, the concentration of intrinsic bulk structural defects becomes 10–50 times lower upon the radiation-induced "ordering".

The analysis of the experimental data obtained and those found in the literature allowed us to represent the function $\tau(t)$ graphically, as is shown in Fig. 3. Three intervals can be distinguished in this curve:

1) the interval at the initial stage of irradiation, when the lifetime of defects diminishes, starting from the value τ_0 which corresponds to the lifetime of defects before irradiation to the minimal value which is characterized by a parity between the efficiency of defect gettering and recombination, on the one hand, and that of their generation, on the other hand;

2) the interval of the further increase of the defect lifetime, when the efficiency of defect generation becomes

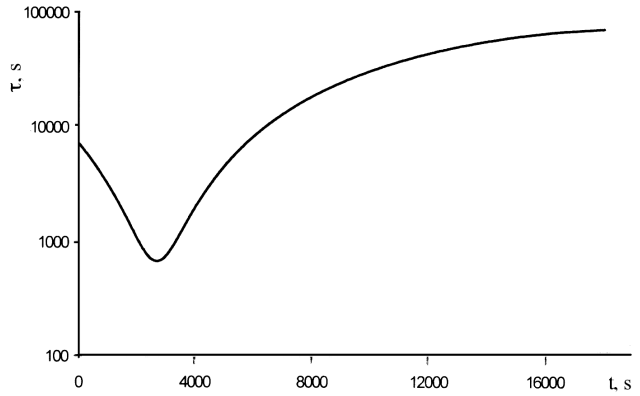

Fig. 3. Dependence of the lifetime of defects on the irradiation dose

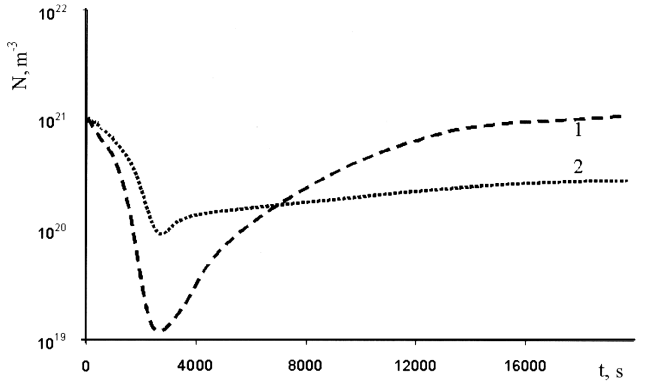

Fig. 4. Dependence of the Cd_i concentration on the irradiation time in the bulk of the specimen (*1*) and on its surface (*2*)

higher than the total efficiency of their recombination and gettering;

3) the interval which is characterized by a dominating role of the generation of defects in the radiation field.

To avoid various complications while solving the diffusion equation, we have tabulated the dependence $\tau(t)$ and, dealing with the relevant equation, considered the value of τ instantaneous. The results of the modeling of processes, taking into account the coefficient of radiation-induced diffusion, are shown in Fig. 4. On the basis of the results obtained, the following conclusions can be drawn:

— a pronounced difference is observed between the variation regularities of the Cd_i concentration in the bulk of the crystal and in its near-surface layer (about 1000 atomic layers in thickness) at the initial stage of irradiation: the bulk concentration of defects decreases more rapidly than that in the near-surface layer;

— if the absorbed irradiation dose increases, the bulk concentration starts to increase rapidly, while the near-surface one practically does not change.

The experimental results correlate well with the data that were obtained when analyzing the radiation-induced modifications of the defect concentration profiles in the crystal bulk and in the near-surface regions. Two curves (see Fig. 4) clearly demonstrate the characteristic minima of the defect concentration, when the crystals have absorbed the irradiation dose of about 750 R, which corresponds to the irradiation time of about 3000 s. These minima correspond to the maximal radiation-induced ordering of the crystal structure, namely: the maxima of the current carrier mobility and the electroconductivity, provided the dose of 750 R and a fixed concentration; the saturation of the effective density of surface states; the saturation of the direct current in the current-voltage characteristic; and a reduction of the characteristic maximum in the capacitor-voltage characteristics down to the background level.

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ДО МОДЕЛІ РАДІАЦІЙНО-СТИМУЛЬОВАНОГО ВПОРЯДКУВАННЯ ДЕФЕКТНОЇ СТРУКТУРИ КРИСТАЛІВ CdS

Б.В. Павлик, М.В. Лишак

Р е з ю м е

Запропоновано фізичну і математичну моделі процесу радіаційно-стимульованого впорядкування дефектної структури кристалів CdS. В основу моделі покладено процеси гетерування дефектів (Cd_i) на стоках з врахуванням суттєвого (приблизно на 2 порядки) збільшення коефіцієнта дифузії дефектів в полі дії радіації, а також збільшення часу життя дефектів при дозах опромінення до 750 Р.