SELF-CONSISTENT DEFORMATION-DIFFUSION SPATIAL REDISTRIBUTION OF DEFECTS IN A SEMICONDUCTOR INDUCED BY THE ELECTRIC FIELD

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A nonlinear model describing the self-consistent electric-deformation-diffusion redistribution of point defects in semiconductors has been proposed. Conditions for the bulk of a CdTe semiconductor to be purified from clusters of ionized Cd_i interstitials have been established.

1. Introduction

Semiconductors belonging to A^2B^6 group have recently found a wide use as materials for ionizing radiation detectors, solar cells, laser screens, and electron-optical modulators [1]. Semiconductor crystals contain a certain number of point defects at temperatures $T > 0$. Additional defects are generated under the influence of external factors: heating, deformation, particle irradiation, and so on. Semiconductor crystals can be subjected to external factors purposefully at definite stages of a technological cycle aimed at creating a semiconductor device (irradiation, introduction of impurities, control over the relationship between compound component fluxes during the epitaxial growth). On the other hand, such an influence can be undesirable; for instance, if the device operates under enhanced radiation conditions. The presence of charged point defects in a semiconductor is one of the reasons for the ageing and degradation of semiconductor-based devices. In particular, the presence of defects brings about a modification of $p-n$-junction characteristics and the formation of uncontrollable conducting channels. This affects the operation stability of ionizing radiation sensors fabricated on the basis of A^2B^6 semiconductors [1, 2].

In work [2], the analysis of a possibility for charged point defects with the average concentration of about 10^{15} cm^{-3} to be the redistributed in a CdS semiconductor, when the latter is placed into an electric field, was done. It was demonstrated that, in the electric field $E = 6\times10^4$ V/cm, the concentration of interstitial Cd_i in the CdS semiconductor bulk can be reduced by 4 orders of magnitude.

However, under the action of intense irradiation, the point defects (interstitial atoms and vacancies) in significant concentrations ($N_d > 10^{17}$ cm^{-3}) are created in a semiconductor material. If the concentration of defects exceeds a certain critical value, their interaction with the self-consistent deformation field gives rise to the formation of ordered defection-deformation structures: clusters and periodic structures [3–6]. In this case, the problem of finding the spatial redistribution of the concentration $N_d(x)$ of charged point defects in the semiconductor under the action of an electric field has to be solved in a self-consistent way, taking the deformation effects into account.

In this work, a model of the self-consistent electric-deformation-diffusion redistribution of charged defects in A^2B^6 semiconductors has been developed, and the conditions for the CdTe semiconductor bulk to be purified from clusters created by ionized Cd_i interstitial atoms have been established.

2. Model

Let a semiconductor that contains point defects with average concentration N_{d0} be placed into an electric field which is applied to the electrodes at the specimen ends. Defects interact with both the electric field $E = -\frac{d\varphi(x)}{dx}$, where $\varphi(x)$ is the electrostatic potential, and the deformation field $U(x) = \frac{\partial u_x}{\partial x}$, where u_x is the component of the medium displacement vector. The expression for the free energy density in the semiconductor crystal looks like

$$F = \frac{1}{2}\rho c_l^2 U^2(x) + \frac{1}{3}\rho c_l^2 \alpha U^3(x) + \frac{1}{4}\rho c_l^2 \beta U^4(x) +$$
$$+\rho c_l^2 l_0^2 \frac{\partial^2 U(x)}{\partial x^2} U(x) - \theta_d l_d^2 N_d(x) \frac{\partial^2 U(x)}{\partial x^2} -$$
$$-\theta_d N_d(x) U(x) + Ze\varphi(x) N_d(x) - TS, \quad (1)$$

where ρ is the medium density, c_l is the longitudinal sound velocity, $\theta_d = K_A \Delta\Omega$ is the deformation potential, $\Delta\Omega$ is a variation of the crystal volume induced by a defect, K_A is the uniform elastic constant, l_d and l_0 are the characteristic lengths of the interaction between defects and crystal atoms, and between atoms, respectively, α and β are the constants of elastic anharmonicity [4], T is the temperature, and S is the entropy. Here, the elastic energy of an imperfect crystal with anharmonic terms (the first, second, and third terms), the interaction of lattice atoms with one another (the fourth term) and with defects (the fifth term), the potential energy of interaction between defects and lattice deformation (the sixth term), and the energy of electrostatic interaction between defects and the electric field are taken into consideration. Below, we consider defects as once ionized donors, i.e. $Z = 1$.

Taking into account that

$$\sigma(x) = \frac{\partial F}{\partial U(x)}, \tag{2}$$

we find the expression for the stress $\sigma(x)$ in the defect structure which include anharmonic terms [4]:

$$\sigma(x) = \rho c_l^2 U(x) - \rho c_l^2 |\alpha| U^2(x) + \rho c_l^2 \beta U^3(x) +$$

$$+\rho c_l^2 l_0^2 \frac{\partial^2 U(x)}{\partial x^2} - \theta_d N_d(x). \tag{3}$$

The equation for a deformation, $\rho \frac{\partial^2 U(x)}{\partial t^2} = \frac{\partial^2 \sigma(x)}{\partial x^2}$, in the stationary case with regard for Eq. (3) reads

$$c_l^2 \frac{\partial^2 U(x)}{\partial x^2} + c_l^2 l_0^2 \frac{\partial^4 U(x)}{\partial x^4} - c_l^2 |\alpha| \frac{\partial^2 (U^2(x))}{\partial x^2} +$$

$$+c_l^2 \beta \frac{\partial^2 (U^3(x))}{\partial x^2} - \frac{\theta_d}{\rho} \frac{\partial^2 N_d(x)}{\partial x^2} = 0. \tag{4}$$

Besides the ordinary diffusion flux of defects, the action of deformation and electric fields invokes an additional flux $j_d = \upsilon N_d$, where

$$\upsilon = \frac{D\theta_d}{kT} \left(\frac{\partial U(x)}{\partial x} + l_d^2 \frac{\partial^3 U(x)}{\partial x^3} \right) - \mu \frac{\partial \varphi(x)}{\partial x}.$$

The first term is the velocity of defects that appears due to the deformation gradient in the semiconductor (D is the diffusion coefficient, and k the Boltzmann constant), and the second term is the drift velocity of charged defects in the electric field (μ is the mobility of defects). Making allowance for the additional flux, the diffusion equation looks like

$$D \frac{\partial^2 N_d}{\partial x^2} - \frac{D\theta_d}{kT} \frac{\partial}{\partial x} \left(N_d(x) \left(\frac{\partial U(x)}{\partial x} + l_d^2 \frac{\partial^3 U(x)}{\partial x^3} \right) \right) +$$

$$+\frac{\partial}{\partial x} \left(N_d(x) \mu \frac{\partial \varphi(x)}{\partial x} \right) = 0. \tag{5}$$

The integration of Eq. (5) brings about the formula for the spatial distribution of the concentration of point defects:

$$N_d(x) = N_{d0} e^{\frac{\theta_d}{kT} \left(U(x) + l_d^2 \frac{\partial^2 U(x)}{\partial x^2} \right) + E_0 - \frac{\mu}{D} \varphi(x)}. \tag{6}$$

Here, the constant E_0 can be found from the condition

$$\int_{-\frac{L}{2}}^{\frac{L}{2}} N_d(x) dx = N_{d0} L, \tag{7}$$

where L is the crystal length.

The electrostatic potential $\varphi(x)$ is determined from the Poisson equation

$$\nabla^2 \varphi(x) = -\frac{e}{\varepsilon\varepsilon_0} (N_d(x) - n(\mathrm{x})) \tag{8}$$

with the boundary conditions $\varphi\left(-\frac{L}{2}\right) = \varphi_0$ and $\varphi\left(\frac{L}{2}\right) = 0$, where ε is the dielectric permittivity of the medium, and $n(x)$ is the electron concentration that satisfies the equation

$$D_n \frac{d^2 n(x)}{dx^2} - \frac{d}{dx} \left(n(x) \mu_n \frac{d\varphi}{dx} \right) = 0, \tag{9}$$

where D_n and μ_n are the diffusion coefficient and the mobility of electrons, respectively.

Let us present the deformation and the concentration of defects in the form

$$U(x) = U_0 + U_l(x); N_d(x) = N_{d0} + N_{dl}(x), \tag{10}$$

where $U_l(x)$ and $N_{dl}(x)$ are the spatially non-uniform components of the deformation and the defect concentration, respectively, and $U_0 = \frac{\theta_d}{K_A} N_{d0}$ is the spatially averaged deformation. Substituting expression (6) for the spatial distribution of the point defect concentration into Eq. (4) and using the approximation $\frac{\theta_d}{kT} \left(U(x) + l_d^2 \frac{\partial^2 U(x)}{\partial x^2} \right) \ll 1$, we obtain the inhomogeneous nonlinear differential equation for the medium deformation

$$c_l^2 \frac{\partial^2 U(x)}{\partial x^2} + c_l^2 l_0^2 \frac{\partial^4 U(x)}{\partial x^4} - c_l^2 |\alpha| \frac{\partial^2 \left(U^2(x)\right)}{\partial x^2} +$$

$$+c_l^2\beta\frac{\partial^2\left(U^3(x)\right)}{\partial x^2}-\frac{\theta_d^2}{\rho kT}\times$$

$$\times\frac{\partial^2\left(N_{d0}e^{E_0-\frac{\mu}{D}\varphi(x)}\left(U(x)+l_d^2\frac{\partial^2 U(x)}{\partial x^2}\right)\right)}{\partial x^2}=$$

$$=\frac{\theta_d}{\rho}N_{d0}\frac{\partial^2\left(e^{E_0-\frac{\mu}{D}\varphi(x)}\right)}{\partial x^2}. \qquad (11)$$

Averaging the electrostatic potential $\varphi(x)$ over the crystal length and taking expression (10) into account, we obtain an equation that is similar to Eq. (11a) from work [4],

$$\frac{\partial^2 U_l(x)}{\partial x^2}-aU_l(x)+fU_l^2(x)-cU_l^3(x)=0 \qquad (12)$$

with the coefficients renormalized by the electric field:

$$a=\frac{1-\frac{N_{d0}}{N_{dc}}\chi}{l_d^2\frac{N_{d0}}{N_{dc}}\chi-l_0^2};\quad f=\frac{|\alpha|}{l_d^2\frac{N_{d0}}{N_{dc}}\chi-l_0^2};\quad c=\frac{\beta}{l_d^2\frac{N_{d0}}{N_{dc}}\chi-l_0^2}.$$

Here,

$$N_{dc}=\frac{\rho c_l^2 kT}{\theta_d^2};\quad \chi=\frac{\frac{\mu EL}{2D}}{e^{\frac{\mu EL}{2D}}-1+\frac{2\mu E\sqrt{a_0}}{D}\frac{N_{d0}}{N_{dc}}}$$

$$E=\frac{\varphi_0}{L};\quad a_0=\frac{1-\frac{N_{d0}}{N_{dc}}}{l_d^2\frac{N_{d0}}{N_{dc}}-l_0^2}.$$

Equation (12) has a spatially uniform solution which becomes unstable, if the defect concentration exceeds a certain critical value. In this case, a new spatially non-uniform stationary state emerges. Depending on the magnitude of the average concentration of point defects, the solution of Eq. (12) looks like

$$U_l(x)=0,\quad N_{d0}<N_{dc1}, \qquad (13)$$

$$U_l(x)=\text{sign}\theta_d\frac{A}{B+sh(-\sqrt{a}x)},\quad N_{dc1}<N_{d0}<N_{dc2}, \qquad (14)$$

$$U_l(x)=\text{sign}\theta_d\frac{A}{B+ch(\sqrt{a}x)},\quad N_{dc2}<N_{d0}<N_{dc}, \qquad (15)$$

$$U_l(x)=\text{sign}\theta_d\frac{A}{B+\sin(\sqrt{|a|}x)},\quad N_{d0}>\frac{N_{dc}}{\chi}, \qquad (16)$$

where $A=3\sqrt{2}\,|a|\left(\left|9ca-2f^2\right|\right)^{-1/2}$, $N_{dc1}=\frac{N_{dc}}{\chi}\left(\frac{l_0}{l_d}\right)^2$, $B=f\sqrt{2}\left(\left|9ca-2f^2\right|\right)^{-1/2}$, $N_{dc2}=\frac{N_{dc}}{\chi}(1-\frac{2\alpha^2}{9\beta})$, and $\frac{2\alpha^2}{9\beta}=\frac{4}{9}$ [4].

The electrostatic potential is determined from Eq. (9) with the use of the electroneutrality condition, $n(x)=N_d(x)$. The deviation from electroneutrality approximation is found with the help of the Poisson equation.

By substituting formulas (13)–(16) into expression (6), we obtain the spatial distribution of the point defect concentration in an external electric field at various average concentrations of defects N_{d0}.

3. Results of Calculations and Their Discussion

Calculations were carried out for a CdTe semiconductor with the spatially uniform concentration of interstitial cadmium $N_{d0}=6\times10^{19}$ cm^{-3} with the following parameters: $T=600$ °C, $D=3\times10^{-9}$ cm^2/s [2], $D_n=10^2$ cm^2/s, $\mu_n=10^3$ cm^2/(V × s) [1], $\theta_d=10$ eV, $\varepsilon=9.7$, $l_0=0.5$ nm, $l_d=2.9$ nm [4], $\rho c_l^2=0.79$ Mbar, $K_A=450$ eV/nm^3 [7], and $L=1$ μm.

Consider the case where there is a symmetric cluster of interstitial cadmium Cd_i in the semiconductor CdTe [formula (15)]. The results of calculations of the spatial redistribution of Cd_i defects in self-consistent electric and deformation fields are depicted in Fig. 1 for various electric field strengths.

Let the average concentration of point defects be in the range 10^{18} cm^{-3} $<N_{d0}<10^{20}$ cm^{-3}. If the external electric field is absent, there exists a cluster of interstitial Cd_i defects in the semiconductor CdTe. The application of the electric field violates the cluster symmetry; namely, the concentration of donors decreases in the near-anode region, and, on the contrary, their accumulation near the cathode is observed.

The self-consistent electric-deformation-diffusion redistribution of ionized Cd_i donors in the electric field is governed by two factors: 1) their interaction with the elastic medium, which causes the emergence of the deformation defect flux $j\sim\frac{\partial U}{\partial x}$, and 2) the drift of ionized donors in the external electric field. If the electric field strength is low, $E<10^4$ V/cm, the dominant role is played by the first factor, and there is an asymmetric cluster of interstitial Cd_i defects in the semiconductor bulk. If the electric field strength grows, a reduction of

the defect concentration in the cluster limits is observed (Fig. 1).

In the absence of external electric field, the cluster size $d_{\text{cluster}} = \frac{1}{\sqrt{a_0}}$ is about 3 nm for the average concentration of point defects $N_{d0} = 6 \times 10^{19}$ cm^{-3}. The growth of the electric field strength is accompanied by a monotonous reduction of the cluster dimensions,

$$d_{\text{cluster}}(E) = \frac{1}{\sqrt{a}} = l_d \sqrt{\frac{\frac{N_{d0}}{N_{dc}}\chi(E) - \frac{l_0^2}{l_d^2}}{1 - \frac{N_{d0}}{N_{dc}}\chi(E)}}.$$

The cluster size is defined by the characteristic radius of the interaction between defects and atoms, l_d. It depends on the electric field strength, the average concentration of defects, and the elastic constants of the semiconducting material. If the condition

$$\frac{N_{d0}}{N_{dc}} \frac{\frac{\mu EL}{2D}}{e^{\frac{\mu EL}{2D}} - 1 + \frac{2\cdot\mu\sqrt{a_0}E}{D}\frac{N_{d0}}{N_{dc}}} < \left(\frac{l_0}{l_d}\right)^2$$

is satisfied, the cluster formed by interstitial cadmium in the CdTe bulk disappears.

In addition, we may predict that a semiconductor-based device intended to operate under conditions of intense irradiation would be more stable with respect to the emergence of defect-deformation structures (clusters and periodic structures), if it would operate in an external electric field. This is related to an increase of the critical concentrations of defects, above which the processes of formation of defect-deformation structures occur. The growth of threshold concentrations, at which the defect-deformation structures arise, is connected with a decrease of the elastic constants of a semiconducting material that is placed into an external electric field.

4. Conclusions

1. Conditions of purifying a semiconducting material from a defect cluster under the influence of an electric field have been determined. It is demonstrated that the cluster of interstitial Cd_i in the CdTe semiconductor bulk disappears, if the strength of the applied electric field exceeds 60 kV/cm.

2. The dependence of the size of an interstitial atom cluster on the external electric field strength has been studied. It is shown that the electric field growth is accompanied by a monotonous reduction of the cluster size.

3. It is shown that the critical concentration of defects, above which self-organized defect-deformation

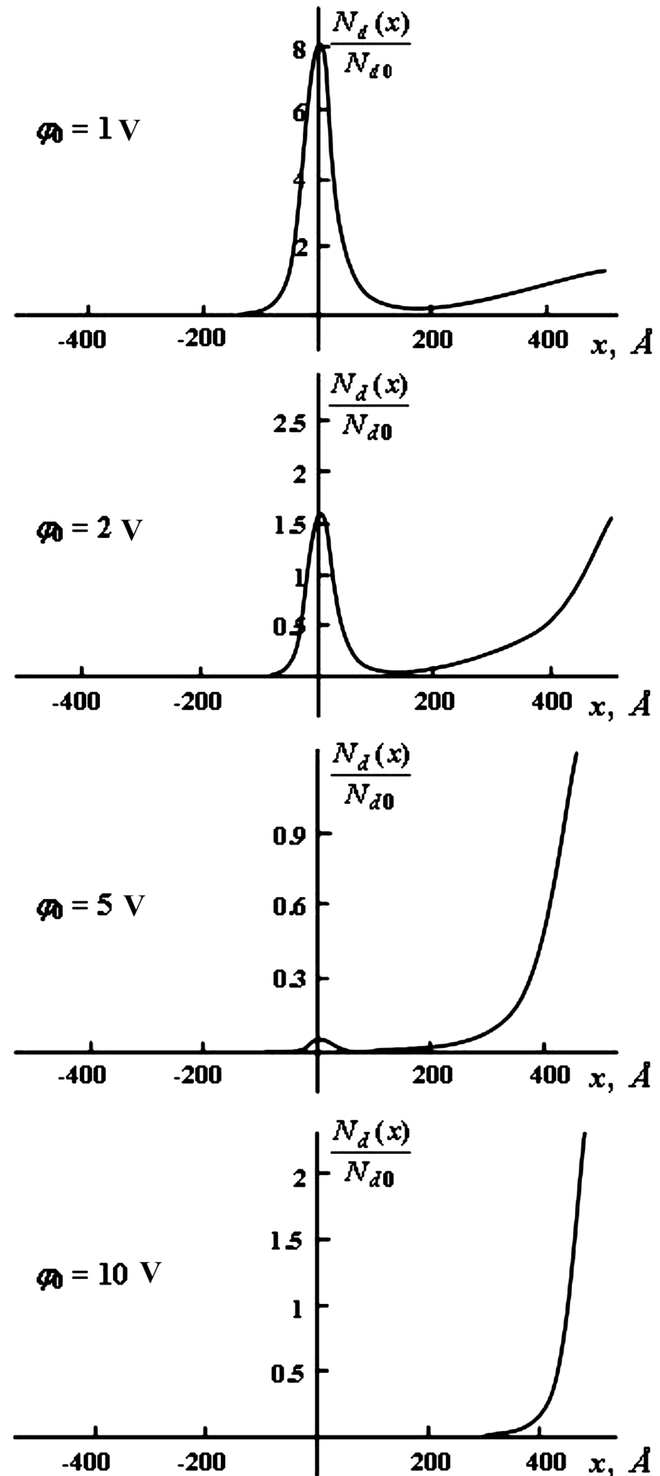

Fig. 1. Spatial distribution of the Cd^+ ion concentration for various voltages applied to the CdTe semiconductor which contains a cluster of interstitial Cd_i defects

structures are formed in the semiconductor, increases with the external electric field strength.

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САМОУЗГОДЖЕНИЙ ДЕФОРМАЦІЙНО-ДИФУЗІЙНИЙ ПРОСТОРОВИЙ ПЕРЕРОЗПОДІЛ ДЕФЕКТІВ У НАПІВПРОВІДНИКУ ПІД ДІЄЮ ЕЛЕКТРИЧНОГО ПОЛЯ

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Р е з ю м е

Побудовано нелінійну модель самоузгодженого електро-деформаційно-дифузійного перерозподілу точкових дефектів у напівпровідниках. Встановлено умови очищення об'єму напівпровідника CdTe від кластерів, утворених іонізованим міжвузловинним Cd_i.