INFLUENCE OF DEFORMATION EFFECTS ON ELECTRICAL PROPERTIES OF METAL–SEMICONDUCTOR–DOPED SEMICONDUCTOR STRUCTURE

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The influence of elastic deformations that arise owing to a mismatch between the lattice parameters of contacting semiconductor materials and in a vicinity of the defect cluster induced by interstitial cadmium in a doped semiconductor CdTe substrate on the electron injection into the insulating layer of the metal–undoped $Zn_xCd_{1-x}Te$ semiconductor–n-CdTe semiconductor substrate structure has been studied.

1. Introduction

Recently, when developing semiconductor devices, contacts between metal and semiconductor with an intermediate undoped i-layer [1] have got a wide application, in particular, for the detection of high-frequency signals [2] and the fabrication of high-voltage pulse $p - i - n$ diodes [3].

In work [4], a self-consistent analytical solution was obtained in the diffusion-drift approximation for the problem of charge carrier injection into a finite-thickness insulating i-layer in metal–i-layer–heavily doped semiconductor substrate structures. The approach proposed by the authors takes into account both bulk effects, which are associated with the current confinement by a space charge, and contact phenomena at the boundaries of the undoped semiconductor i-layer. However, the model proposed by the authors of work [4] does not make allowance for the influence of deformation effects, which can be considerable in the cases where a mismatch between the lattice parameters of contacting semiconductor materials (CdTe/ZnTe, GaAs/InAs) is large (up to 6–7%), and the concentration of point defects is high ($N_d > 10^{17}$ cm^{-3}).

As was shown in works [5–8], when the concentration of defects (interstitial atoms and vacancies) exceeds some critical value, their interaction with the self-consistent field of deformation gives rise to a formation of ordered defect-deformation structures (clusters and periodic structures). The presence of defect clusters in semiconductor materials substantially affects their electrophysical and optical properties. In particular, as was shown in works [9, 10], clusters of interstitial Cd_i's are fast channels of recombination in CdS. In work [8], conditions for purifying the CdTe semiconductor bulk from clusters formed by ionized interstitial Cd_i were found, and the influence of an external electric field on the cluster size was analyzed.

Owing to the self-consistency of the electron-deformation coupling, a non-uniform deformation, which emerges due to the presence of defect clusters and the mismatch between the lattice parameters of contacting materials in metal–i-layer–heavily doped semiconductor structures, results in considerable modifications of spatial distributions of charge carrier concentration, electrostatic potential $\varphi(x)$, and electric field $E(x)$; which is reflected, in particular, in current-voltage characteristics (CVCs) of such structures. An important matter is how to predict the variation of electric properties under the influence of mechanical stresses and how to establish conditions, under which the influence of external factors that change a strained state of the semiconductor structure on electric properties would be minimal.

In this work, the electrostatic potential, electric field strength, conduction electron concentration $n(x)$, and CVCs of the metal–undoped $Zn_xCd_{1-x}Te$ semiconductor–n-CdTe semiconductor substrate (metal$-i-n^+$) structure have been calculated with regard for elastic deformations that arise both owing to a mismatch between the lattice parameters of contacting semiconductor materials and in the defect cluster vicinity in a doped CdTe semiconductor substrate.

2. Model

Consider a three-layer structure: metal–undoped $Zn_xCd_{1-x}Te$ layer with thickness L–doped n^+-CdTe semiconductor substrate. The coordinate x is reckoned

from the metal–semiconductor interface into the semiconductor depth.

1. Let the semiconductor substrate ($x \geq L$) contain point defects with the average concentration N_{d0}. Defects interact with both the electric field $E = -\frac{d\varphi(x)}{dx}$ and the strain field $U(x) = \frac{\partial u_x}{\partial x}$, where u_x is the component of the medium displacement vector. Since the substrate thickness is much larger than that of the undoped i-layer, the substrate deformation resulting owing to the mismatch between the lattice parameters of contacting semiconductor materials can be neglected. Only the elastic strains that are created by point defects—namely, ionized interstitial cadmium in CdTe material—are taken into consideration.

To find the parameter of crystal lattice deformation and the defect concentration, it is necessary to solve the equations [8]

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

$$+ c_l^2 \beta \frac{\partial^2 (U^3(x))}{\partial x^2} - \frac{\theta_d}{\rho} \frac{\partial^2 N_d(x)}{\partial x^2} = 0, \quad (1)$$

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

$$+ \frac{\partial}{\partial x} \left(N_d(x) \mu \frac{\partial \varphi(x)}{\partial x} \right) = 0, \quad (2)$$

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 change of the crystal volume per one defect; K_A is the uniform elastic constant; l_d and l_0 are the characteristic lengths of the defect–crystal atom and atom–atom interactions, respectively; α and β are the constants of elastic anharmonicity; T is the temperature; D is the coefficient of defect diffusion; and k is the Boltzmann constant.

Integrating Eq. (2), we obtain

$$N_d(x) = N_{d0} \exp \left(\frac{\theta_d}{kT} \left(U_l(x) + l_d^2 \frac{\partial^2 U_l(x)}{\partial x^2} \right) - \frac{\mu}{D} \varphi(x) \right) \approx$$

$$\approx N_{d0} \left(1 + \frac{\theta_d}{kT} \left(U_l(x) + l_d^2 \frac{\partial^2 U_l(x)}{\partial x^2} \right) - \frac{\mu}{D} \varphi(x) \right). \quad (3)$$

Substituting Eq. (3) into Eq. (1), we obtain a nonlinear inhomogeneous differential equation for the medium deformation

$$\frac{\partial^2 U_l(x)}{\partial x^2} - a U_l(x) + f U_l^2(x) - c U_l^3(x) =$$

$$= \frac{\frac{N_{d0}}{N_{dc}}}{l_d^2 \frac{N_{d0}}{N_{dc}} - l_0^2} \frac{e\varphi(x)}{\theta_d}, \quad (4)$$

where $U_l(x)$ is the spatially non-uniform component of the deformation,

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

$$c = \frac{\beta}{l_d^2 \frac{N_{d0}}{N_{dc}} - l_0^2}; \quad N_{dc} = \frac{\rho c_l^2 kT}{\theta_d^2}.$$

For a heavily doped n^+-substrate, one can take advantage of the Thomas–Fermi approximation [4]. Then, making allowance for deformation effects, the electrochemical potential looks like

$$\chi_s(x) = \frac{\hbar^2}{2m_s} \left(3\pi^2 n(x)\right)^{2/3} - e\varphi_s(x) + a_c U(x), \quad (5)$$

where m_s is the effective mass of an electron in the doped semiconductor material, $n(x)$ is the electron concentration distribution, and a_c is the constant of the hydrostatic deformation potential of the conduction band.

Let us consider the n^+-layer as a three-component system which contains electrons with the concentration $n(x)$, ionized motionless donors with the concentration N^+, and mobile donors with the concentration $N_d(x)$. The condition

$$n_0 = N^+ + N_{d0}, \quad (6)$$

where n_0 is a spatially uniform value of conduction electron concentration, is evidently fulfilled.

From formula (5), one can determine the charge carrier concentration:

$$n(x) = \left(\frac{2m_s}{\hbar^2} \right)^{3/2} \cdot \frac{\left(\chi_s(x) + e\varphi_s(x) - a_c U(x)\right)^{3/2}}{3\pi^2}. \quad (7)$$

The current density is

$$j = \frac{\sigma}{e} \frac{d\chi_s}{dx}, \quad (8)$$

where σ is the specific conductance of the n^+-layer. Let us assume that the conductivity of the doped substrate to be high enough, so that the condition $\frac{j}{\sigma} e L_s \ll \chi_0$, where L_s is the substrate thickness, and $\chi_0 = \chi(\infty) = \frac{\hbar^2}{2m_s} \left(3\pi^2 n_0\right)^{2/3} + a_c U_0$, is satisfied. Then the electron concentration can be presented, in the linear approximation, as follows:

$$n(x) = n_0 + R\left(e\varphi_s(x) - a_c U_l(x)\right), \quad (9)$$

where $R = \left(\frac{2m_s}{\hbar^2}\right)^{3/2} \frac{\sqrt{\chi_0}}{2\pi^2}$.

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

$$\nabla^2 \varphi_s(x) = -\frac{e}{\varepsilon_s \varepsilon_0}\left(N_d(x) + N^+ - n(\mathrm{x})\right), \tag{10}$$

where ε_s is the dielectric permittivity of a semiconductor substrate material.

Therefore, having solved the system of equations (4) and (10), where expressions (3) and (9) are taken into account, one can obtain the spatial distributions of electrostatic potential, $\varphi_s(x)$, crystal lattice deformation, $U_l(x)$, conduction electron concentration, $n(x)$, and defects, $N_d(x)$, in the doped semiconductor substrate. Let us solve this system using the iteration method. In the first approximation, we obtain the solution of Eq. (4) taking no interaction between defects and the electrostatic field into account ($\varphi_s(x) = 0$). Depending on the magnitude of average point defect concentration, the solution of Eq. (4) looks like

$$U_l(x) = 0, \quad N_{d0} < N_{dc1}, \tag{11}$$

$$U_l(x) = \frac{A \operatorname{sign}\theta_d}{B + \operatorname{sh}\left(-\sqrt{a}\,(x - x_0)\right)}, \quad N_{dc1} < N_{d0} < N_{dc2}, \tag{12}$$

$$U_l(x) = \frac{A \operatorname{sign}\theta_d}{B + \operatorname{ch}\left(\sqrt{a}\,(x - x_0)\right)}, \quad N_{dc2} < N_{d0} < N_{dc}, \tag{13}$$

$$U_l(x) = \frac{A \operatorname{sign}\theta_d}{B + \sin\left(\sqrt{|a|}\,(x - x_0)\right)}, \quad N_{d0} > N_{dc}, \tag{14}$$

where x_0 means the position of a cluster in the doped semiconductor substrate, $A = 3\sqrt{2}\,|a|\left|9ca - 2f^2\right|^{-1/2}$, $B = \sqrt{2}f\left|9ca - 2f^2\right|^{-1/2}$, $N_{dc1} = N_{dc}\left(\frac{l_0}{l_d}\right)^2$, $N_{dc2} = N_{dc}\left(1 - \frac{2\alpha^2}{9\beta}\right)$, and $\frac{2\alpha^2}{9\beta} = \frac{4}{9}$ [6].

Below, we confine the consideration to the case of symmetric defect cluster, which corresponds to formula (13). Substituting Eqs. (3) and (9) into the Poisson equation (10) and taking Eq. (6) into account, we obtain the following spatial distribution of the electrostatic potential in the doped semiconductor substrate:

$$\varphi_s(x) = C_1 e^{-gx} - \frac{1}{2\mathrm{g}} e^{gx} \int f(x) e^{-gx} dx +$$

$$+\frac{1}{2g} e^{-gx} \int f(x) \cdot e^{gx} dx, \tag{15}$$

where

$$f(x) = W U_l(x) + \left(W - \frac{g_0^2 a_c}{e}\right) l_d^2 \frac{\partial^2 U_l(x)}{\partial x^2},$$

$g_0 = \sqrt{\frac{e^2 R}{\varepsilon_s \varepsilon_0}}$, $g = \sqrt{\frac{e^2\left(R + \frac{N_{d0}}{kT}\right)}{\varepsilon_s \varepsilon_0}}$, and C_1 is the integration constant.

2. Let us write down the expressions for the electrochemical potential and the electric current density, as well as the Poisson equation, for the undoped i-layer, when a deformation of the crystal lattice is taken into consideration 4:

$$\chi(x) = kT \ln \frac{n(x)}{N_i} + \Delta_i - e\varphi(x) + a_c U(x), \tag{16}$$

$$j = n\mu_n \frac{d\chi}{dx}, \tag{17}$$

$$\nabla^2 \varphi(x) = \frac{e}{\varepsilon \varepsilon_0} n(\mathrm{x}), \tag{18}$$

where $N_i = 2\left(\frac{2\pi m kT}{h^2}\right)^{3/2}$ is the effective density of states, Δ_i is the gap between the conduction bands at the semiconductor interface, μ_n is the electron mobility, and ε is the relative dielectric permittivity of the medium. From Eqs. (16)–(18) and bearing in mind that $E = -\frac{d\varphi(x)}{dx}$, we obtain a nonlinear equation for the electric field,

$$\frac{kT}{e}\frac{d^2 E}{dx^2} + E\frac{dE}{dx} + \frac{a_c}{e}\frac{dE}{dx}\frac{dU}{dx} = -\frac{j}{\mu_n \varepsilon \varepsilon_0}. \tag{19}$$

Consider the case where the distance from the interface between semiconductor materials to the center of a cluster of defects that are contained in the substrate is much larger than the cluster size ($x_0 \gg 1/\sqrt{a}$). In this case, a deformation in the i-layer, which arises in a vicinity of defect-deformation structures, can be neglected. However, a deformation of the undoped layer induced by a mismatch between the lattice parameters of contacting materials can be substantial. To study the influence of this mismatch on the electron injection into the undoped layer, we confine ourselves to the linear approximation for the deformation,

$$U(x) = U_0 \frac{x}{L}, \tag{20}$$

$U_0 = U_{xx} + U_{yy} + U_{zz},$

$$U_{yy} = U_{zz} = \frac{a_s - a_0}{a_s}, U_{xx} = -\frac{2C_{12}}{C_{11}} U_{yy},$$

where U_{xx}, U_{yy}, and U_{zz} are the components of the strain tensor; a_s and a_0 are the lattice parameters of the substrate and i-layer materials, respectively.

Changing over to dimensionless quantities and integrating Eq. (19), we obtain

$$\frac{d\tilde{E}}{dz} + \frac{\tilde{E}^2}{2} + \tilde{j}z = A, \tag{21}$$

where A is an integration constant, $\tilde{E} = \frac{e}{kTg_0}\left(E + \frac{a_c U_0}{eL}\right)$, $\tilde{j} = \frac{e^2 j}{\varepsilon\varepsilon_0 \mu_n (kT)^2 g_0^3}$, and $z = g_0 x$.

The solution of Eq. (21) can be expressed in terms of Airy functions and looks like [4]

$$\tilde{E}(z) = -2\left(\frac{\tilde{j}}{2}\right)^{1/3} \frac{Ai'(y) + C_2 \cdot Bi'(y)}{Ai(y) + C_2 \cdot Bi(y)}, \tag{22}$$

where $y(z) = \left(\tilde{j}/2\right)^{1/3}\left(A/\tilde{j} - z\right)$.

In order to calculate the electric field, electrostatic potential, and current density, let us take advantage of a technique proposed in work [4]. The following conditions, which enable the integration constants to be determined as functions of the current density, must be satisfied at the interface between semiconductor materials:

$$\begin{cases} \varphi(L-0) = \varphi_s(L+0); \\ \varepsilon \frac{d\varphi}{dx}\left.\right|_{x=L-0} = \varepsilon_s \frac{d\varphi_s}{dx}\left.\right|_{x=L+0}; \\ \chi(L-0) = \chi_s(L+0). \end{cases} \tag{23}$$

Equating the electrochemical potential of the semiconductor at its interface with the metal to $\chi(0)$, we obtain an additional boundary condition

$$n(0) = N_i e^{-\frac{\Delta}{kT}}, \tag{24}$$

where $\Delta = \Delta_i - e\varphi(0) - \chi(0)$ is the potential barrier height at the semiconductor–metal interface.

In view of Eq. (18), equality (24) can be rewritten in the form

$$\left.\frac{d^2\varphi}{dx^2}\right|_{x=0} = \frac{eN_i}{\varepsilon\varepsilon_0} e^{-\frac{\Delta}{kT}}. \tag{25}$$

Then, taking into account that $\chi(0) = \chi_0 - eV$ [4], where V is the applied voltage, we obtain the expression

$$eV = e\varphi(0) + \chi_0 + \Delta - \Delta_i. \tag{26}$$

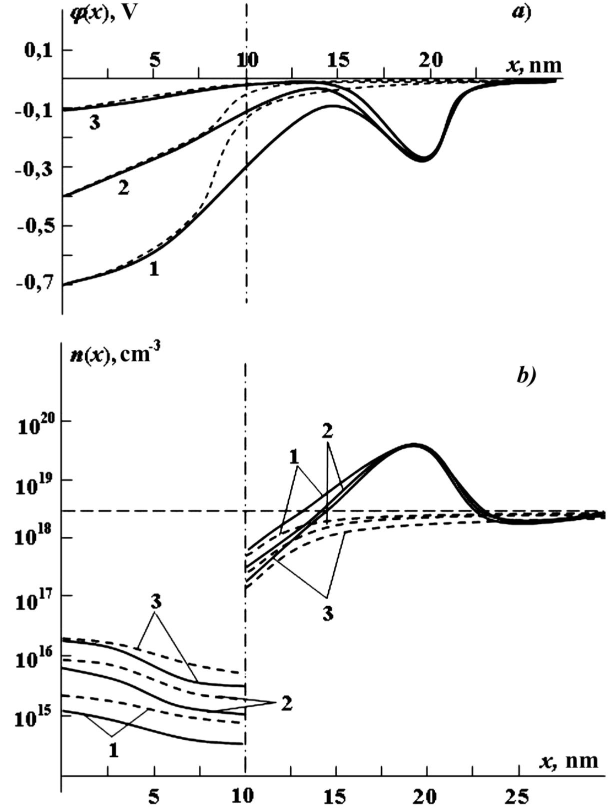

Fig. 1. Spatial distributions of the electrostatic potential (a) and electrons (b) in the metal–i–n^+ structure with a cluster (solid curves) and without it (dashed curves) for $\Delta = 0.6$ eV (*1*), 0.3 eV (*2*), and 0 eV at $\Delta_i = 0$ eV (*3*)

By solving the system of equations (23) and (25), we can determine $\varphi(0)$ as a function of the current density. Substituting it into Eq. (26), we obtain a transcendental equation which allows the CVC of the structure under investigation to be determined.

3. Calculation Results and Their Discussion

In Fig. 1, the results of calculations of the spatial distributions of electrostatic potential and conduction electron concentration in the metal–undoped CdTe–doped n-CdTe substrate structure at the zero bias voltage are presented for the following values of parameters: $T = 300$ °C, $D = 3 \times 10^{-9}$ cm^2/s [11], $a_c = 3.38$ eV, $D_n = 10^2$ cm^2/s, $\mu_n = 10^3$ cm^2/(V × s) [12], $\theta_d = 10$ eV, $\varepsilon = \varepsilon_s = 9.7$, $l_0 = 0.5$ nm, $l_d = 2.9$ nm [6], $\rho c_l^2 = 0.79$ Mbar, $K_A = 450$ eV/nm^3 [13], $x_0 = 20$ nm, $L = 10$ nm, $N_{d0} = 2 \times 10^{18}$ cm^{-3}, and $n_0 = 3 \times 10^{18}$ cm^{-3}. The calculations were carried out for various Δ-values

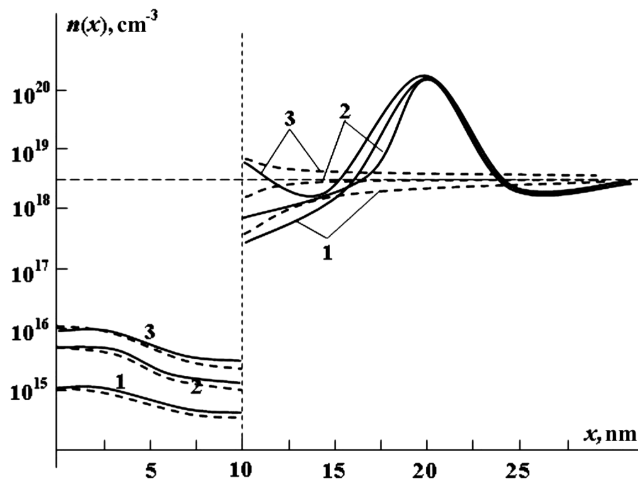

Fig. 2. Spatial distributions of electrons in the metal–i–n^+ structure at $\Delta_i = 0.3$ eV and for $\Delta = 0.3$ (*1*), 0.6 (*2*), and 0 eV (*3*). The dashed curve corresponds to calculations taking no deformation effects into account

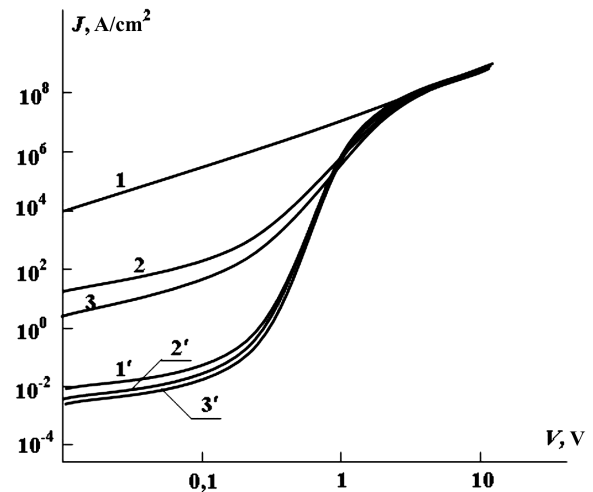

Fig. 3. Current-voltage characteristics of the metal–i–n^+ structure at various values of the average defect concentration ($\Delta_i = 0$): $N_{d0} = 0$ (*1*, *1′*), 2×10^{18} (*2*, *2′*), and 6×10^{18} cm^{-3} (*3*, *3′*). $\Delta = 0$ (*1*, *2*, *3*) and 0.3 eV (*1′*, *2′*, *3′*)

within the interval 0 eV $\leq \Delta \leq$ 0.6 eV. The height Δ of the barrier at the interface with the metal can be reduced (even down to zero) by the δ-doping of the i-layer immediately near the metal [2, 4].

Let us consider the case where a symmetric cluster is formed by interstitial cadmium Cd_i in a CdTe semiconductor substrate, and let its center be located at the point x_0 (formula (13)). The presence of the cluster invokes a non-uniform internal electric field in the bulk of doped CdTe and a corresponding redistribution of charge carriers. Some localization of electrons is observed in a vicinity of the defect-deformation structure and, accordingly, a reduction of their concentration in the i-layer. The influence of deformation effects on the charge carrier injection becomes more substantial, if the barrier Δ at the interface with the metal decreases. For instance, at $\Delta = 0$, owing to the presence of the interstitial Cd_i cluster in the substrate, the concentration of electrons in the i-layer becomes four times lower (Fig. 1).

In the case where $Zn_xCd_{1-x}Te$ is used as an intermediate layer between the metal and the substrate material, an additional barrier Δ_i arises at the interface between semiconductors due to the gap that occurs between the conduction bands in contacting materials. In this case (Fig. 2), the influence of deformation effects leads to an insignificant (up to 20%) increase of the electron concentration in the i-layer near the interface between the semiconductors. This phenomenon is associated with the fact that the barrier at the semiconductor interface considerably reduces the influence of defect-deformation structures existing in the doped substrate on the charge carrier injection. The mismatch between the lattice parameters of contacting semiconductors results in the emergence of a non-uniform tensile deformation in the i-layer and, accordingly, an additional electron flux from the metal contact to the i-layer–doped semiconductor interface.

In Fig. 3, the CVCs of metal–i-layer–doped semiconductor substrate structures are exhibited for various Δ and average defect concentrations N_{d0}. The presence of clusters in the substrate brings about a substantial reduction of the electric current at insignificant bias voltages. An increase of the applied voltage leads to a decrease of the cluster size [8]. Therefore, the current densities at high voltages ($V > 1$ V) practically do not differ from the corresponding values in the defect-free structure. If the defect concentration increases (Fig. 3), the current density diminishes. This can be explained by the fact that a tensile deformation grows in a vicinity of the cluster, whereas an increase of the electron concentration in the doped substrate practically does not influence the injection of carriers into the i-layer.

4. Conclusions

The influence of a deformation that arises in a vicinity of the defect cluster of interstitial cadmium in a doped CdTe semiconductor substrate on the injection of electrons into the insulating layer of the metal–i–n^+ struc-

ture has been studied. In the absence of a barrier at the metal–semiconductor interface, the presence of the cluster is demonstrated to result in a reduction of the charge carrier concentration in the i-layer by a factor of four.

The mismatch between the lattice parameters of the contacting semiconductor substances in the metal–i–n^+ structure is found to be the origin of the electron concentration growth in the i-layer.

The increase of barriers at both the metal–semiconductor and semiconductor–semiconductor interfaces is shown to reduce the influence of the cluster on the charge carrier injection into the i-layer of the metal–i–n^+ structure.

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ВПЛИВ ДЕФОРМАЦІЙНИХ ЕФЕКТІВ НА ЕЛЕКТРИЧНІ ВЛАСТИВОСТІ СТРУКТУРИ МЕТАЛ–НАПІВПРОВІДНИК–ЛЕГОВАНИЙ НАПІВПРОВІДНИК

Р.М. Пелещак, О.В. Кузик, О.О. Даньків

Р е з ю м е

Досліджено вплив пружних деформацій, що виникають як за рахунок невідповідності параметрів ґраток контактуючих напівпровідникових матеріалів, так і в околі кластера дефектів міжвузловинного кадмію у легованій напівпровідниковій підкладці CdTe, на інжекцію електронів в ізолюючий шар структури метал–нелегований напівпровідник $Zn_xCd_{1-x}Te$–напівпровідникова підкладка n-CdTe.