
INFLUENCE OF ELECTRON-DEFORMATION INTERACTION ON THE ELECTRIC PROPERTIES OF A BARRIER AT AN EDGE DISLOCATION

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In the framework of a self-consistent model of the electron-deformation interaction, the influence of the filling factor of the conduction band on the rectification parameters of a dislocation barrier has been studied. It has been shown that the basic characteristics of the diode effect at a single edge dislocation are governed by both the electrostatic potential of the charged dislocation and the self-consistent potential of the electron-deformation interaction, resulting from the spatial redistribution of conduction electrons in the vicinity of the dislocation.

($n_0 \approx 10^{17} \div 10^{19} \text{ cm}^{-3}$). So that, while calculating the electric properties of the dislocation barrier, the electron-deformation mechanism of charge carrier screening should be made allowance for, in addition to the Debye and Read ones.

Therefore, this work is aimed at studying the influence of the electron-deformation mechanism of charge carrier screening on the current-voltage characteristics (CVCs) of the dislocation barrier.

1. Introduction

Studying the electric properties of a barrier at an edge dislocation is challenging for the analysis of the dislocation-induced modifications of the electron state spectrum in the semiconductor, as well as for finding the efficient opportunities to use the diode effect produced by this barrier in microelectronic devices. These properties were substantiated theoretically in the framework of the model of the electrostatic field related to a charged dislocation [1]. In works [2,3], the rectification properties of a microcontact between metal and n -silicon at the end of a 60° dislocation have been discovered experimentally.

However, in heavily doped semiconductor crystals with edge dislocations – such as CdTe, $\text{Cd}_{1-x}\text{Zn}_x\text{Te}:\text{Cl}$ [4], and $\text{Sm}_{1-x}\text{Cd}_x\text{S}$ ($0.15 \leq x \leq 0.22$) [5] – there is a significant concentration of conduction electrons

2. Calculations of the CVC of an Edge Dislocation in a Semiconductor

One of the effects that demonstrate the violation of local neutrality in semiconductor crystals in the vicinity of dislocations is the asymmetry of CVCs in the case where the current flows from the dislocation axis to the semiconductor periphery and vice versa [1,3,6]. Relevant experiments designed to study a separate dislocation in silicon [1] or germanium [7] crystals evidence for the presence of the diode effect.

Owing to the self-consistent electron–deformation coupling, the local spatial redistribution of conduction electrons in the vicinity of the edge dislocation gives rise to the emergence of the electron-deformation electrostatic potential $\varphi_{\text{el-def}}(\rho, \theta)$ [8], which has not been taken into account in works [1, 9] while calculating the CVC of a separate charged dislocation in semiconductors.

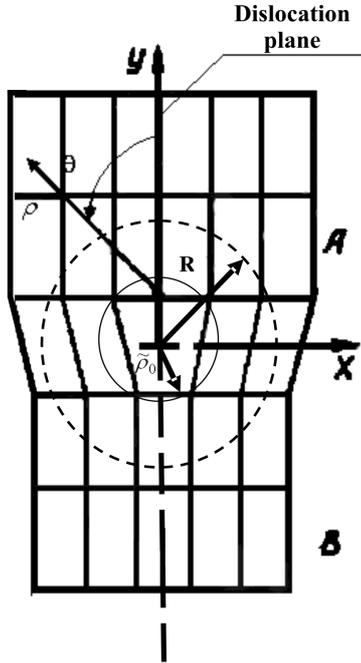


Fig. 1. Geometry of a single crystal with an edge dislocation

Consider that the dislocation core coincides with the Z -axis of a cylindrical coordinate system (Fig. 1), and the vector of the stationary current density $\vec{j}(\vec{\rho})$ is directed radially, so that $\text{div } \vec{j} = 0$ and

$$j(\vec{\rho}) = \frac{j_0 \tilde{\rho}_0}{\rho}. \tag{1}$$

Here, $\tilde{\rho}_0$ is the minimal distance, at which the diffusion approximation for the current density remains eligible. In the region $\rho < \tilde{\rho}_0$, the diffusion approximation does not hold true. But, in this case, the electron becomes captured onto a dislocation level, and

$$j(\vec{\rho}) = \mu n(\rho) \nabla \zeta(\vec{\rho}), \tag{2}$$

where μ is the electron mobility, $\zeta(\vec{\rho})$ and $n(\rho)$ are the local values of the chemical potential and the concentration, respectively, of electrons in the semiconductor's bulk.

We assume that the difference between the chemical potentials for electrons located on the dislocation core and far from it (i.e. at a distance $\rho \geq R$, where R is the Read radius, which determines the screening radius of the dislocation electric field), is equal to eU : $\zeta(0) - \zeta(R) = eU$, where U is the applied voltage, and $\zeta(0)$ and $\zeta(R)$ are the chemical potentials on the dislocation line and at a distance of the Read cylinder

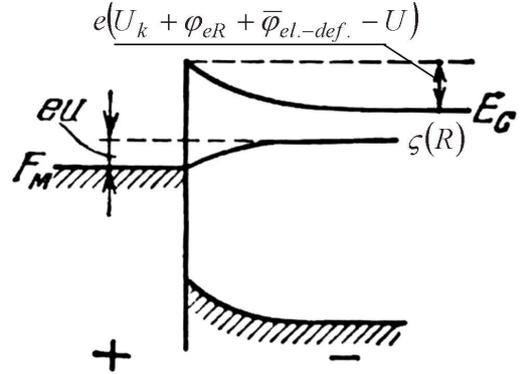


Fig. 2. Current rectification at the metal–semiconductor contact

radius (Fig. 2). Then, Eqs. (1) and (2) can be written down as follows:

$$\frac{j_0 \tilde{\rho}_0}{\rho} = \mu n(\rho) \nabla_\rho \zeta(\rho),$$

$$j_0 = \frac{1}{\tilde{\rho}_0} \mu \rho n(\rho) \nabla_\rho \zeta(\rho),$$

$$eU \equiv \zeta(R) - \zeta(0) = \frac{j_0 \tilde{\rho}_0}{\mu} \int_{\tilde{\rho}_0}^R \frac{d\rho}{\rho n(\rho)},$$

$$j_0 = \frac{eU\mu}{\tilde{\rho}_0} \frac{1}{\int_{\tilde{\rho}_0}^R \frac{d\rho}{\rho n(\rho)}}. \tag{3}$$

The explicit expression for the dependence $n(\rho)$ is determined by the structure of the chemical potential $\zeta(\rho)$ in the Boltzmann statistics approximation for electrons in the bulk of an n -type semiconductor with the donor concentration n_d and the diffusion coefficient D :

$$\nabla_\rho \zeta = e \nabla_\rho \varphi(\rho) + e \nabla_\rho \bar{\varphi}_{el-def}(\rho) + kT n^{-1} \nabla_\rho n,$$

$$\mu = \frac{eD_e}{kT}. \tag{4}$$

The system of equations (1), (2), and (4) yields

$$n(\rho) = \exp \left[-\frac{e(\varphi_{eR}(\rho) + \bar{\varphi}_{el-def}(\rho))}{kT} \right] \times \left\{ n_d - \frac{j_0 \tilde{\rho}_0}{D_e} \int_{\tilde{\rho}_0}^R \frac{d\rho}{\rho} \exp \left[\frac{e(\varphi_{eR}(\rho) + \bar{\varphi}_{el-def}(\rho))}{kT} \right] \right\}, \tag{5}$$

where $\varphi_{eR}(\rho)$ is the electrostatic component of the potential around a charged edge dislocation in the Read approximation [6],

$$\varphi_{eR}(\rho) = -\frac{2ef}{\varepsilon a} \left[\ln\left(\frac{R}{\rho}\right) - \frac{1}{2} \left(1 - \frac{\rho^2}{R^2}\right) \right],$$

$$\pi R^2 n_d = \frac{f}{a}. \quad (6)$$

Here, $f = a/c$ is the filling factor for dislocation levels, which indicates how shorter the distance between “dangling” bonds (its value is of the order of the lattice constant) is in comparison with the interval between filled states; ε is the relative static dielectric constant; R is the radius of the Read cylinder, provided that $R > \rho_D$; $\rho_D^2 = \frac{\varepsilon kT}{4\pi e^2 n_d}$; a is the interatomic distance;

$$\bar{\varphi}_{\text{el-def}}(\rho) = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} \varphi_{\text{el-def}}(\rho, \theta) d\theta \quad (7)$$

is the electron–deformation component of the edge–dislocation potential [10];

$$\varphi_{\text{el-def}}(\rho, \theta) = -\frac{2D|S|}{\rho_0 e} I_1(g\rho_0) K_1(g\rho) \cos\theta, \quad (8)$$

$$g^2 = \frac{e^2 R_S}{\varepsilon \varepsilon_0};$$

$$R_S = \left(\frac{3}{8}\right)^{1/3} \frac{1}{\alpha^* \pi^{4/3} \Omega_0^{1/3}} \frac{n_0^{1/3} [1 + pn_0^{1/3}]^{1/2}}{1 - \frac{3}{2} pn_0^{1/3} [1 + pn_0^{1/3}]^{1/2}}, \quad (9)$$

$$p = \frac{S^2}{(3\pi^2)^{2/3} \alpha^* K}, \quad (10)$$

$$D = \frac{1 - 2\nu}{2\pi(1 - \nu)} b, \quad (11)$$

and ρ_0 is the radius of the dislocation core.

Substituting Eq. (8) into Eq. (7) and integrating the result, we obtain

$$\bar{\varphi}_{\text{el-def}}(\rho) = -\frac{4D|S|}{e\rho_0\pi} I_1(g\rho_0) K_1(g\rho), \quad (12)$$

where $I_1(g\rho_0)$ and $K_1(g\rho)$ are the Bessel and McDonald functions, respectively [11]. To within a logarithmic accuracy in the parameter $g\tilde{\rho}_0 \geq 1$,

$$K_1(g\rho) \approx \ln\left(\frac{2}{g\rho}\right). \quad (13)$$

Expressions (1)–(6) link the quantities j_0 and f , and expressions (6) and (12) do the quantities U and f to each other. In order to derive the formula which would describe the CVC, i.e. to find the relation between j_0 and U , we must express the factor of dislocation filling f in terms of the quantities E_d and U . For this purpose, we write down the equation for the chemical potential $\zeta(R)$,

$$-E_d + eU + V_c + \bar{V}_{\text{el-def}} = \zeta(R), \quad (14)$$

where

$$V_c = -e\varphi_{eR}\left(\frac{a}{f}\right), \quad \bar{V}_{\text{el-def}} = -e\bar{\varphi}_{\text{el-def}}\left(\frac{a}{f}\right),$$

E_d is the energy of the dislocation level in the energy gap of the semiconductor reckoned from the bottom of the conduction band, $\zeta(R) \equiv E_F$ is the value of the chemical potential at distances far from the dislocation, and the quantity $\varphi(\rho)$ is taken from Eq. (6).

Calculating the integral $\int_{\tilde{\rho}_0}^R \frac{d\rho}{\rho n(\rho)}$ in formula (3) makes the system of equations (3)–(6), (12), and (14) substantially simpler. As a result, we have

$$j_0 = \frac{eD_e n_d}{\tilde{\rho}_0} \frac{1 - \exp\left(-\frac{eU}{kT}\right)}{\int_{\tilde{\rho}_0}^R \frac{d\rho}{\rho} \exp\left[\frac{e(\varphi_{eR}(\rho) + \bar{\varphi}_{\text{el-def}}(\rho))}{kT}\right]}. \quad (15)$$

This formula establishes the relation between the current density j_0 through the dislocation barrier (a Schottky barrier of cylindrical symmetry) and the applied voltage U . It is similar to the expression for the CVC in the diffusion theory of rectification [12], because the charged dislocation can be regarded as a cylindrically symmetric Schottky barrier. The difference consists in that a lower bound is set on the distance from the dislocation axis, i.e. there must be $\tilde{\rho}_0 \leq \rho$; the parameter $\tilde{\rho}_0$ may be the radius of a microprobe’s tip or the radius of the electron capture onto the dislocation level.

To within a logarithmic accuracy in the parameter $\frac{R}{\tilde{\rho}_0} \gg 1$,

$$\varphi_{eR}(\rho) \approx \frac{2ef}{\varepsilon a} \ln \frac{R}{\rho}. \quad (16)$$

Taking Eq. (16) into account, expression (15) reads

$$j_0 = \frac{eD_e n_d}{\tilde{\rho}_0} \left(1 - e^{-\frac{eU}{kT}}\right) \frac{\tilde{\Gamma}}{2\Gamma_1} (g\tilde{\rho}_0)^{\Gamma_1} \left(\frac{\tilde{\rho}_0}{R}\right)^{2\Gamma}, \quad (17)$$

where

$$\tilde{\Gamma} = 2\Gamma + \Gamma_1, \quad \Gamma = \frac{e^2 f}{\varepsilon \varepsilon_0 a k T},$$

$$\Gamma_1(n_0) = \frac{4D|S|}{\rho_0 k T \pi} I_1(g\rho_0), \quad (18)$$

and Γ_1 is the parameter, which describes the screening originated from the electron-deformation interaction.

If the basic characteristics of the diode effect at a single edge dislocation are formed under the influence of the electrostatic and electron-deformation potentials, as well as the contact potential difference emerging at the contact interface between a metal microprobe inserted into the etching hole and the semiconductor (it is the place where a single dislocation ends at the semiconductor's surface), the analytical functional dependence of the current density j_{0M} around the edge dislocation on the voltage applied to the metal-semiconductor system looks like

$$j_{0M} = -j_S \left(1 - \exp\left(-\frac{|e|U}{kT}\right)\right), \quad (19)$$

where

$$j_S = \frac{eD_e n_d}{\tilde{\rho}_0} \frac{\tilde{\Gamma}}{2\Gamma_1} (g\tilde{\rho}_0)^{\Gamma_1} \left(\frac{\tilde{\rho}_0}{R}\right)^{2\Gamma} e^{-\frac{|e|U_k}{kT}} \quad (20)$$

is the saturation current density, $eU_k = \Phi_M - \Phi_{\text{semic}}$ is the contact potential difference, and Φ_M and Φ_{semic} are the thermionic work functions of the metal and the semiconductor, respectively.

As one can see from formulas (17) and (20), the density of the current through the dislocation barrier j_{0M} is determined not only by the Read screening parameter Γ , but by the electron-deformation one Γ_1 as well, whereas the latter was not taken into account in works [1, 3, 6]. In crystals with strong electron-deformation coupling, the inequalities $\frac{e\varphi_{\text{el-def}}}{S\Delta U} \lesssim 1$,

where $S\Delta U$ is the potential energy of an electron in the deformation field and $e\varphi_{\text{el-def}}$ is the corresponding energy in the field of electrostatic potential resulted from the redistribution of the electron concentration owing to the electron-deformation interaction, and

$$\frac{\Gamma_1}{\Gamma} = \frac{4D|S|\varepsilon_0 \varepsilon a I_1(g\rho_0)}{e^2 \rho_0 f} \lesssim 1. \quad (21)$$

are satisfied.

If condition (21) is satisfied, the parameter of the electron-deformation screening Γ_1 is to be taken into account while calculating the CVC of the dislocation barrier (a Schottky barrier at the edge dislocation).

To analyze the influence of the conduction electron concentration n_0 and the constant of the deformation potential S on the nonlinearity of the CVC of a dislocation barrier that emerges near the edge dislocation core, we have to calculate the dependence of the current strength on the voltage applied across the dislocation barrier for various values of n_0 and S .

The strength of the electron current through the dislocation barrier is expressed by the integral

$$\begin{aligned} I &= \iint (\vec{j}_{0M} \cdot d\vec{S}) = \iint j_{0M} dS \cos \theta = \\ &= 4\pi^2 \tilde{\rho}_0^2 \int_0^{\pi/2} \cos^2 \theta d\theta = \pi^3 \tilde{\rho}_0^2 j_{0M}. \end{aligned} \quad (22)$$

Substituting relation (19) for the current density j_{0M} into formula (22), we obtain

$$\begin{aligned} I_{\text{sum}}(n_0, S, U) &= -\pi^3 \tilde{\rho}_0 e D_e n_d \frac{\tilde{\Gamma}}{2\Gamma_1} \times \\ &\times (g\tilde{\rho}_0)^{\Gamma_1} \left(\frac{\tilde{\rho}_0}{R}\right)^{2\Gamma} e^{-\frac{|e|U_k}{kT}} \left(1 - e^{-\frac{eU}{kT}}\right). \end{aligned} \quad (23)$$

In Fig. 3, *a*, the results of numerical calculations of the CVC for the contact between a tungsten microprobe and a spot on the *n*-Si surface, where the edge dislocation ends are presented (the temperature $T = 300$ K). Figure 3, *b* depicts the experimental CVC of the same contact. If the tungsten microprobe tip is put in contact with a dislocation-free area of the *n*-Si surface, the corresponding CVC does not reveal diode properties [1].

Figure 3 demonstrates that an edge dislocation that ends at the *n*-Si surface brings about the pronounced diode properties of the microcontact between the silicon

and the metal. In the simplest model [1], the rectification phenomenon at the contact metal–semiconductor can be explained by the emergence of a barrier at the semiconductor surface, the height of which is equal to the difference between the work functions of the metal and the semiconductor: $eU_k = \Phi_M - \Phi_{\text{semic}}$. In the case of a semiconductor of the n -type, for the gate layer to emerge, it is necessary that the work function of electrons from the metal exceed that from the semiconductor.

The authors of works [1, 3] asserted that the rectification properties of a dislocation diode are formed only under the influence of the electrostatic potential emerging around the charged dislocation (Fig. 3, *a*; dashed curve ($\Gamma_1 = 0$, $\Gamma \neq 0$)), because the difference between the electron work functions of the metal and the semiconductor does not play any important role in the formation of a dislocation barrier.

The comparative analysis of the experimental and theoretical CVCs of the dislocation diode (see the Table) shows that, in the n -Si case, the experimental CVC does not agree with the results of calculations of CVC in the framework of the electrostatic model [3]. This is related to the fact that, while calculating the CVC of a dislocation barrier, the influence of the electron-deformation component of the potential, which governs the profile of the CVC depending on the filling factor of the conduction band, has not been taken into account self-consistently. The parameters used for the calculations were as follows: Fig. 3, *a* – $n_0 = 10^{14} \text{ cm}^{-3}$, $\tilde{\rho}_0 = 45 \text{ \AA}$, $\Gamma = 9.95$, $\Gamma_1 = 1.07$, $S = 4.51 \text{ eV}$, and $m^* = 0.11 m_0$; Fig. 3, *b* – $n_0 = 10^{18} \text{ cm}^{-3}$, $\tilde{\rho}_0 = 45 \text{ \AA}$, $\Gamma = 9.95$, $\Gamma_1 = 5.07$, $S = 4.51 \text{ eV}$, $m^* = 0.11 m_0$, and $\mu = 10^3 \text{ cm}^2/(\text{V} \times \text{s})$. Those values correspond to the relevant parameter of a CdTe single crystal and satisfy the criterion of the diffusion theory of rectification in the Schottky barrier [13], i.e. $\left| \frac{eU_k}{kT} \right| \frac{l}{L_D} = 0.1 \ll 1$, where

$L_D^2 = \frac{\varepsilon \varepsilon_0 kT}{e^2 n_0}$ and $l \approx 5 \times 10^{-9} \mu (\text{cm})$ is the mean free path.

In the framework of our approach to the calculation of the CVC of a dislocation diode (formula (23)), such an influence is made allowance for through the electron-deformation mechanism of charge carrier screening

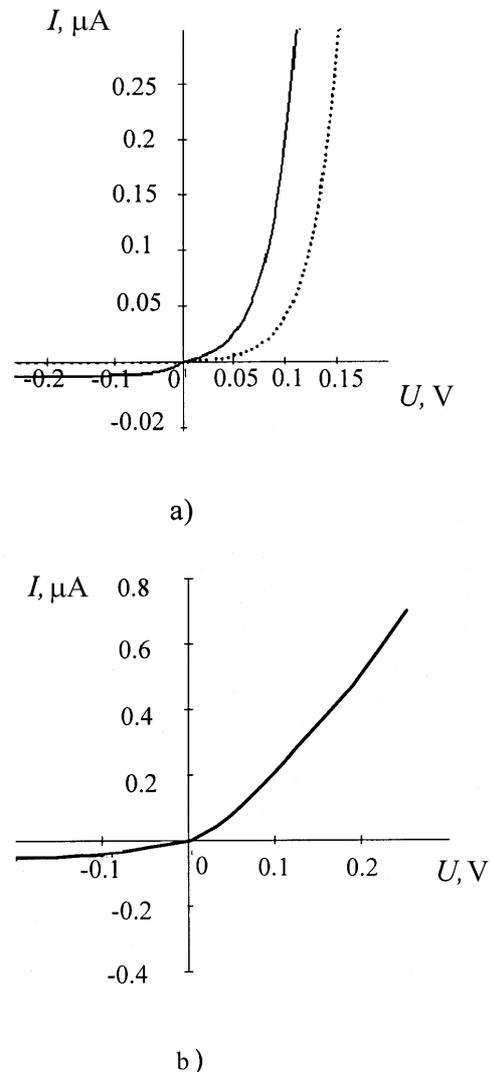


Fig. 3. (a) Calculated CVC for a contact between a tungsten microprobe and n -Si at the edge dislocation end. Dashed curve corresponds to the case $\Gamma_1 = 0$ and $\Gamma \neq 0$. (b) Experimental CVC of the same contact

around the edge dislocation. As a result, in the voltage interval $U = 0.03 \div 0.15 \text{ V}$, the current strength acquires the magnitudes that are practically of the same order as those observed in experiment.

Experimental data and theoretical results for the current-voltage characteristics of a dislocation diode at the interface between n -Si and a tungsten microprobe

$U_{\text{rev}}, \text{ V}$	-0.25	-0.19	-0.125	-0.09	-0.06	-0.03	$U_{\text{fwd}}, \text{ V}$	0.03	0.06	0.09	0.25
$I_{\text{exp}}, \mu\text{A}$	-0.156	-0.051	-0.044	-0.037	-0.28	-0.16	$I_{\text{exp}}, \mu\text{A}$	0.043	0.112	0.196	0.285
$I_{\text{sum}}, \mu\text{A}$	-0.0043	-0.0043	-0.0043	-0.0042	-0.0039	-0.003	$I_{\text{sum}}, \mu\text{A}$	0.0096	0.04	0.14	0.53
$I_{\text{el}}, \mu\text{A}$	-1.88×10^{12}	-1.88×10^{12}	-1.87×10^{12}	-1.8×10^{12}	-1.7×10^{12}	-1.2×10^{12}	$I_{\text{el}}, \mu\text{A} (\Gamma_1 = 0)$	0.0019	0.008	0.0275	0.1

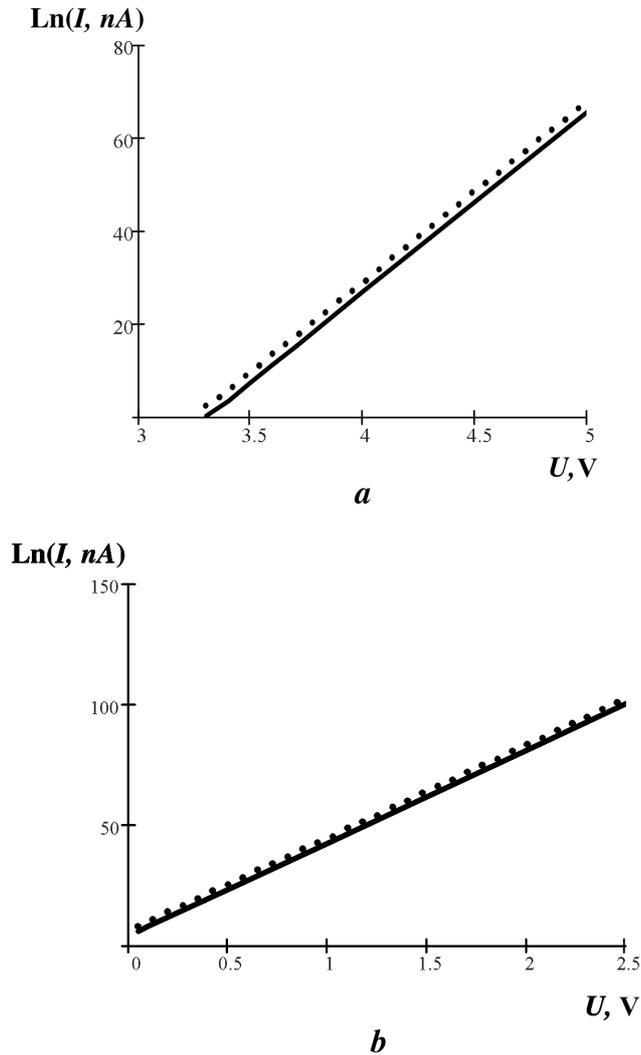


Fig. 4. CVCs for a contact between an indium microprobe and n -CdTe at the edge dislocation end, calculated taking only the electrostatic (dotted curves) or the total (solid curve) potential into account for the conduction electron concentrations $n_0 = 10^{14}$ (a) and 10^{18} cm^{-3} (b)

In Fig. 4, the results of calculations of the CVC of a dislocation barrier taking into account the electron-deformation screening parameter Γ_1 are shown. The contact between a metal (In) microprobe and n -CdTe at the end of the edge dislocation does not give rise to the emergence of rectification properties, since the work function from the metal (In) is lower than that from the n -semiconductor (CdTe).

Therefore, the diode properties are inherent only to the dislocation barrier formed by either the electrostatic potential alone (Fig. 4, dashed curves) or the total

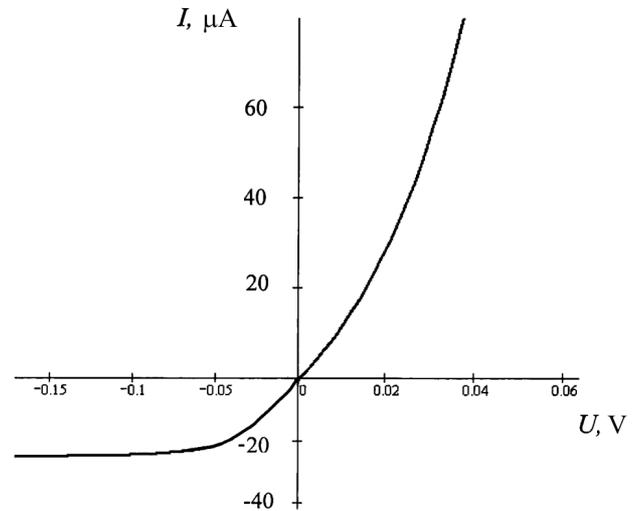


Fig. 5. Calculated CVC for a contact between an indium microprobe and n -CdTe at the edge dislocation end. The calculation parameter are as follows: $n_0 = 10^{18}$ cm^{-3} , $\tilde{\rho}_0 = 45$ Å, $\Gamma = 0$, $\Gamma_1 = 5.07$, $S = 4.51$ eV, $m^* = 0.11 m_0$, and $f = 0$

(electrostatic + electron-deformation) potential (Fig. 4, solid curves). The CVCs obtained demonstrate that, if doping is low ($n_0 \approx 10^{14}$ cm^{-3}), the CVC nonlinearity appears at higher forward voltages than it does at high doping ($n_0 \approx 10^{18}$ cm^{-3}). Figure 4 also demonstrates that the electron-deformation interaction leads to the increase of the dislocation barrier height by 100 meV, if $n_0 \approx 10^{14}$ cm^{-3} , and by 50 meV, if $n_0 \approx 10^{18}$ cm^{-3} .

Figure 5 illustrates the results of our CVC calculations for a dislocation diode, the rectification characteristics of which are formed only at the expense of the electron-deformation barrier (an uncharged edge dislocation). One can see that, even in the case of an uncharged edge dislocation, the diode effects do arise, provided that there is an electron-deformation barrier in the vicinity of the edge dislocation core. The height of such a barrier is lower than the height of the barrier formed under the influence of two potential components, electrostatic and electron-deformation ones. Therefore, the strength of the current, which runs through the dislocation barrier created by the electron-deformation component of the electrostatic potential only is two orders of magnitude larger than that in the case of a charged edge dislocation.

Thus, taking the electron-deformation component $\varphi_{\text{el-def}}$ of the electrostatic potential into account results in that the dislocation barrier possesses rectification properties even in the case of an uncharged edge dislocation.

3. Conclusions

On the basis of our researches, the following conclusions can be drawn:

- the basic characteristics of the diode effect at a single edge dislocation are formed under the influence of both the electrostatic potential of the charged dislocation and the electron-deformation potential which arises as a result of the spatial redistribution of conduction electrons in the vicinity of the dislocation owing to the self-consistent electron–deformation coupling;
- in a semiconductor with strong electron–deformation coupling, an uncharged edge dislocation gives rise to the rectification properties of a contact between this semiconductor and a metal; those properties depend on the deformation potential constant, the filling factor of the conduction band, the elastic constants, and the effective mass of charge carriers.

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ВПЛИВ ЕЛЕКТРОН-ДЕФОРМАЦІЙНОЇ ВЗАЄМОДІЇ НА ЕЛЕКТРИЧНІ ВЛАСТИВОСТІ БАР'ЄРА НА КРАЙОВІЙ ДИСЛОКАЦІЇ

Р.М. Пелещак, М.М. Баран

Резюме

У рамках самоузгодженої електрон-деформаційної моделі досліджено вплив ступеня заповнення зони провідності на випрямні властивості дислокаційного бар'єра. Показано, що основні характеристики діодного ефекту на одиничній крайовій дислокації формуються під впливом як електростатичного потенціалу зарядженої дислокації, так і електрон-деформаційного, зумовленого просторовим перерозподілом електронів провідності в околі дислокації внаслідок самоузгодженого електрон-деформаційного зв'язку.