

# FORMATION OF $n - n^+$ JUNCTIONS IN CRYSTALS WITH SELF-ASSEMBLED DEFECT-DEFORMATION STRUCTURES

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The theory of the formation of double and periodic  $n - n^+$  junctions in crystals with self-assembled defect-deformation structures has been developed.

## 1. Introduction

Making use of external factors (laser irradiation, particle-beam irradiation, and so on), it is possible to generate point defects – interstitial atoms and vacancies – and to control their number by varying the intensity of the radiation source [1, 2]. The interaction between point defects in a crystal and the self-consistent field of deformation caused by them leads to the formation of ordered defect-deformation (DD) structures: clusters and periodic structures [2, 3]. In work [2], the theory describing the formation of a hierarchy of stationary one-dimensional DD structures in an irradiated crystal has been developed. It has been shown that, as the growing spatially homogeneous concentration of defects  $N_{d0}$  exceeds the corresponding threshold values, the stationary localized DD mesostructures are formed first, and the periodic mesostructures afterwards.

This work deals with the study of the formation of  $n - n^+$  junctions in crystals with self-assembled DD structures.

## 2. Theoretical Model

Let the point defects be distributed over the crystal with the average concentration  $N_{d0}$ . The Hamiltonian of this system looks like

$$\hat{H} = \sum_{i\sigma} SU(x_i)c_{i\sigma}^+c_{i\sigma} + \sum_{ij} \sum_{\sigma} \lambda_{ij}^0 c_{i\sigma}^+c_{j\sigma} + \frac{1}{2} \sum_i \rho c_l^2 \Omega_0 U^2(x_i) + \frac{1}{3} \sum_i \rho c_l^2 \Omega_0 \alpha U^3(x_i) +$$

$$+ \frac{1}{4} \sum_i \rho c_l^2 \Omega_0 \beta U^4(x_i) + \sum_i \rho c_l^2 l_0^2 \Omega_0 \frac{\partial^2 U(x_i)}{\partial x_i^2} U(x_i) - \sum_i \theta_d l_d^2 N_d(x_i) \Omega_0 \frac{\partial^2 U(x_i)}{\partial x_i^2} - \sum_i \theta_d N_d(x_i) \Omega_0 U(x_i) + \hat{H}_{\text{Coul}}, \quad (1)$$

where  $S$  is the deformation potential constant of the conduction band,  $c_{i\sigma}^+$  ( $c_{i\sigma}$ ) is the Fermi operator of creation (annihilation) of an electron with spin  $\sigma$  in the localized Wannier state at the  $i$ -th site,  $\lambda_{ij}^0$  are the transfer integrals in the conduction band in the case of a non-distorted lattice,  $\Omega_0$  is the elementary cell volume,  $\rho$  is the density of the medium,  $c_l$  is the longitudinal speed of sound,  $\hat{H}_{\text{Coul}}$  is the energy of Coulomb interaction between electrons,  $\theta_d = K_A \Delta \Omega$  is the deformation potential,  $\Delta \Omega$  is the variation of the crystal volume induced by a single defect,  $K_A$  is the elastic constant under uniform pressure,  $l_d$  is the characteristic radius of interaction between defects and crystal atoms,  $l_0$  is the characteristic radius of interaction of atoms with one another, and  $\alpha$  and  $\beta$  are the constants of elastic anharmonic vibrations [2]. Hamiltonian (1) makes allowance for the shift of the electron level at the  $i$ -th lattice site owing to the deformation  $U(x_i)$  (the first term), the electron overlapping  $\lambda_{ij}^0$  of the  $i$ -th and  $j$ -th sites, the elastic energy of the defect crystal taking the anharmonic terms into account (the third, fourth, and fifth terms), the interaction of lattice atoms with one another (the sixth term) and with defects (the seventh term), the potential energy of interaction between defects and lattice deformation (the eighth term), and the energy of electrostatic interaction between charges.

Using the condition of mechanical balance

$$\left\langle \frac{\partial \hat{H}}{\partial U(x_i)} \right\rangle = \sigma(x_i)V, \quad (2)$$

where  $V$  is the crystal volume, we find the expression for the stress  $\sigma(x)$  in the defect structure which takes the anharmonic terms and those of the electron-deformation interaction into account:

$$\sigma(x) = Sn(x) + \rho c_l^2 U(x) - \rho c_l^2 |\alpha| U^2(x) + \rho c_l^2 \beta U^3(x) + \rho c_l^2 l_0^2 \frac{\partial^2 U(x)}{\partial x^2} - \theta_d N_d(x). \quad (3)$$

Here,  $n(x) = \sum_i \langle c_{i\sigma}^+ c_{i\sigma} \rangle \delta(x - x_i)$  is the spatial distribution of the conduction electron concentration over the non-uniformly deformed crystal, and  $\langle c_{i\sigma}^+ c_{i\sigma} \rangle$  is the electron-electron correlation function [4].

The deformation equation  $\rho \frac{\partial^2 U(x)}{\partial t^2} = \frac{\partial^2 \sigma(x)}{\partial x^2}$ , taking Eq. (3) into account, reads

$$\frac{\partial^2 U(x)}{\partial t^2} = \frac{S}{\rho} \frac{\partial^2 n(x)}{\partial x^2} + c_l^2 \frac{\partial^2 U(x)}{\partial x^2} + c_l^2 l_0^2 \frac{\partial^4 U(x)}{\partial x^4} - c_l^2 |\alpha| \frac{\partial^2 (U^2(x))}{\partial x^2} + c_l^2 \beta \frac{\partial^2 (U^3(x))}{\partial x^2} - \frac{\theta_d}{\rho} \frac{\partial^2 N_d(x)}{\partial x^2}. \quad (4)$$

The equation that describes the concentration of defects looks like

$$\frac{\partial N_d}{\partial t} = D_d \frac{\partial^2 N_d}{\partial x^2} - \frac{D_d \theta_d}{kT} \times \frac{\partial}{\partial x} (N_d (\frac{\partial U}{\partial x} + l_d^2 \frac{\partial^3 U}{\partial x^3})) + G_d - \frac{N_d}{\tau_d}, \quad (5)$$

where  $G_d$  is the generation rate of point defects, and  $\tau_d$  is their lifetime. The recombination of defects is neglected in this consideration ( $\tau_d^{-1} = 0$ ).

In the stationary case, by solving the system of equations (4) and (5), we obtain the following nonlinear equation for the self-consistent deformation:

$$\frac{\partial^2 U_l}{\partial x^2} - a U_l + f U_l^2 - c U_l^3 - p \frac{S}{\rho c_l^2} n(x) = 0. \quad (6)$$

Here,  $U_l(x) = U(x) - U_0$  is the spatially nonuniform part of the deformation,  $U_0 = \frac{\theta_d}{K_A} N_{d0}$  is the averaged deformation,  $a = (1 - N_{d0}/N_{dc}) D^{-1}$ ,  $f = |\alpha|/D$ ,  $c = \beta/D$ ,  $D = l_d^2 N_{d0}/N_{dc} - l_0^2$  [2],  $p = D^{-1}$ , and  $N_{dc} = \rho c_l^2 kT/\theta_d^2$  is the critical concentration of defects.

The self-consistent diffusion- and deformation-induced redistribution of defects in the crystal gives rise to the emergence of an inhomogeneous distortion. Such a distortion in the crystal with point defects, owing to

the self-consistent electron-deformation coupling, brings about the spatial redistribution of conduction electrons  $\Delta n(x)$  and the emergence of the electrostatic potential  $\varphi(x)$  in the vicinity of DD structures [5, 6]. To find  $\Delta n(x)$  and  $\varphi(x)$ , the following self-consistent system of equations is to be solved:

1) the stationary Schrödinger equation

$$\left[ \nabla_x^2 - \frac{S}{\alpha^*} U(x) + \frac{e}{\alpha^*} \varphi(x) \right] \Psi_n(x) = -\frac{1}{\alpha^*} (\lambda_n - \lambda_0) \Psi_n(x), \quad (7)$$

where  $\alpha^* = \hbar^2/(2m^*)$ , and  $\lambda_0$  is the bottom energy of the conduction band in a nondeformed crystalline matrix; 2) the equation which determines the concentration of electrons

$$n(x) = \sum_n \frac{\Psi_n^*(x) \Psi_n(x)}{\exp\left(\beta \left(\tilde{\lambda}_n - \mu\right)\right) + 1}, \quad (8)$$

where  $\tilde{\lambda}_n = \lambda_n - \lambda_0$ ;

3) the Poisson equation which determines the electrostatic potential  $\varphi(x)$ ,

$$\nabla^2 \varphi(x) = -\frac{e}{\varepsilon \varepsilon_0} \Delta n(x), \quad (9)$$

where  $\varepsilon$  is the dielectric permittivity of the medium; and 4) the equation for the chemical potential

$$\frac{\Omega_0}{V} \int_V n(x) dV = \bar{n}, \quad 0 \leq \bar{n} \leq 2, \quad (10)$$

where  $\bar{n} = n_0 \Omega_0$  is the preset average number of electrons at a lattice site.

In this work, we consider the crystals with a substantial concentration of conduction electrons  $n = (10^{17} \div 10^{20}) \text{ cm}^{-3}$  (doped semiconductors of the  $n$ -type and metals). Under those conditions, provided that the deformation is non-uniform, the redistribution of conduction electrons induced by a shift of the conduction band and a local change of its width gives rise to the considerable charge accumulation, so that the energy of the electrostatic interaction becomes of the same order as the deformation energy  $SU$  [5], i.e.  $e|\varphi| \sim SU$ . In this case, a plane wave is a good approximation for the solution of the Schrödinger equation (7).

In the linear approximation, the variation of the conduction electron concentration in the vicinity of a

self-assembled cluster is determined by the relationship [6]

$$\Delta n = R_S(e\varphi - SU), \quad (11)$$

where  $R_S$  is a function that depends on the population of the conduction band by electrons, the elastic constants, the effective mass of current carriers, and the deformation potential constant of the conduction band. Taking Eq. (11) into account, the deformation equation (6) and the Poisson equation (9) acquire the forms

$$\frac{\partial^2 U_l}{\partial x^2} - \tilde{a}U_l + fU_l^2 - cU_l^3 = p \frac{S^2 R_S}{\rho c_l^2} \frac{e\varphi}{S}, \quad (12)$$

and

$$\Delta\varphi(x) - g_S^2\varphi(x) = -\frac{Sg_S^2}{e}U_l(x), \quad (13)$$

respectively, where  $\tilde{a} = a - p \frac{S^2 R_S}{\rho c_l^2}$  and  $g_S^2 = \frac{e^2 R_S}{\varepsilon \varepsilon_0}$ . If the electron-deformation interaction is neglected ( $R_S = 0$ ), Eq. (12) coincides with Eq. (11a) from work [2]. The system of equations (12) and (13) is solved by using the iteration method. As the first approximation, the expression for the deformation  $U_l(x)$  is searched at  $R_S = 0$ . Then, depending on the magnitude of the spatially uniform concentration of defects  $N_{d0}$ , the expression for the self-consistent deformation  $U_{0l}(x)$  of the lattice with the spatial distribution of defects  $N_d(x)$ , in the first approximation, looks like [2]

$$U_{0l}(x) = \text{sign}\theta_d \frac{A}{B + \text{sh}(-\sqrt{a}x)}, \quad N_{dc1} < N_{d0} < N_{dc2}, \quad (14)$$

$$U_{0l}(x) = \text{sign}\theta_d \frac{A}{B + \text{ch}(\sqrt{a}x)}, \quad N_{dc2} < N_{d0} < N_{dc}, \quad (15)$$

$$U_{0l}(x) = \text{sign}\theta_d \frac{A}{B + \text{sin}(\sqrt{|a|x})}, \quad N_{d0} > N_{dc}, \quad (16)$$

where

$$A = 3\sqrt{2}|a| (|9ca - 2f^2|)^{-\frac{1}{2}},$$

$$B = \sqrt{2}f (|9ca - 2f^2|)^{-\frac{1}{2}},$$

$$N_{dc1} = N_{dc} \left( \frac{l_0}{l_d} \right)^2,$$

$$N_{dc2} = N_{dc} \left( 1 - \frac{2\alpha^2}{9\beta} \right), \quad \frac{2\alpha^2}{9\beta} = 4/9.$$

The solution of Eq. (13) is

$$\varphi(x) = -\frac{Sg_S}{2e}e^{gsx} \int U_l(x) e^{-gsx} dx + \frac{Sg_S}{2e}e^{-gsx} \times \\ \times \int U_l(x) e^{gsx} dx + C_1 e^{gsx} + C_2 e^{-gsx}, \quad (17)$$

where the constants  $C_1$  and  $C_2$  are to be determined from the boundary conditions.

In the next iteration for  $U_l(x)$ , the solution of the inhomogeneous nonlinear differential equation (12) is tried in the form  $U_l(x) = U_{0l}(x) + U_{1l}(x)$ , where  $U_{1l}(x)$  is found from the equation

$$\frac{\partial^2 U_{1l}}{\partial x^2} - \tilde{a}U_{1l} + fU_{1l}^2 + 2fU_{0l}U_{1l} - cU_{1l}^3 - \\ - 3cU_{0l}^2U_{1l} - 3cU_{0l}U_{1l}^2 = p \frac{S^2 R_S}{\rho c_l^2} \left( \frac{e\varphi}{S} - U_{0l} \right). \quad (18)$$

Since the deformation parameter  $U_l(x) < 1$ , in order to estimate the solution  $U_{1l}(x)$ , we neglect the quadratic and cubic terms. Then,  $U_{1l}(x)$  looks like

$$U_{1l}(x) = \frac{\sqrt{\tilde{a}}S^2 R_S}{2g_S \rho c_l^2} \left[ e^{-\sqrt{\tilde{a}}x} \int \left( e^{gx} \int U_{0l}''(x) e^{-gx} dx - \right. \right. \\ \left. \left. - e^{-gx} \int U_{0l}''(x) e^{gx} dx \right) e^{\sqrt{\tilde{a}}x} dx - \right. \\ \left. - e^{\sqrt{\tilde{a}}x} \int \left( e^{gx} \int U_{0l}''(x) e^{-gx} dx - \right. \right. \\ \left. \left. - e^{-gx} \int U_{0l}''(x) e^{gx} dx \right) e^{-\sqrt{\tilde{a}}x} dx \right]. \quad (19)$$

The relative errors for the potential  $\varphi(x)$  and the deformation parameter  $U_l(x)$  calculated in the first and second iterations do not exceed 1%. Therefore, the first approximation is enough for further calculations.

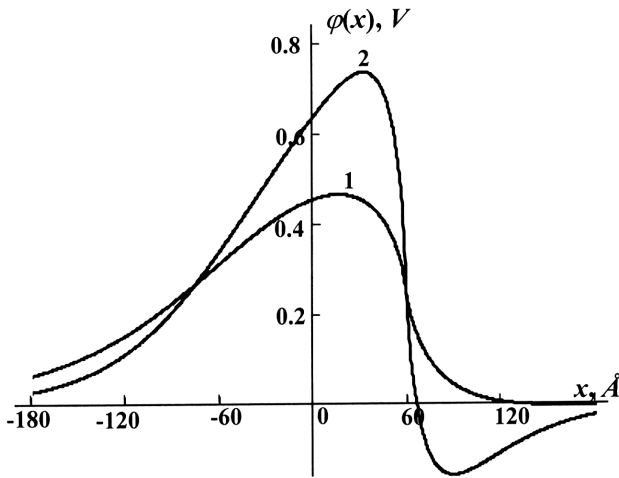


Fig. 1. Coordinate dependences of the electrostatic potential for various average values of the electron concentration  $n_0 = 2.6 \times 10^{17}$  (1) and  $1.6 \times 10^{19} \text{ cm}^{-3}$  (2). The point defect concentration  $N_{d0} = 0.5 \times N_{dc}(1 + (l_0/l_d)^2)$

### 3. Results of Calculations and their Discussion

Calculations were carried out for GaAs crystals with the following parameters:  $\alpha^* = 164.6 \text{ eV} \times \text{\AA}^2$ ,  $S = 7.16 \text{ eV}$ ,  $\rho c_l^2 = 0.79 \text{ eV}/\text{\AA}^3$ ,  $l_0 = 5 \text{ \AA}$ ,  $l_d = 29 \text{ \AA}$ ,  $\theta = 10 \text{ eV}$ , and  $N_{dc} = 10^{20} \text{ cm}^{-3}$ . The anharmonic elastic constant  $\alpha$  was evaluated by the formula  $\alpha = -2\gamma_\Gamma E/(3\rho c_l^2)$ , where  $E = 0.538 \text{ eV}/\text{\AA}^3$  is the Young modulus, and  $\gamma_\Gamma = 0.8$  is the Grüneisen coefficient [7].

Provided that the defect concentration  $N_{d0} < N_{dc1}$ , the internal electric field is absent, because there is no process of defect self-assembling [2]. As a result, there is no spatial redistribution of conduction electrons ( $\Delta n(\vec{r}) = 0$ ), and the formation of an  $n - n^+$  junction is impossible under those conditions.

In the range of the point defect concentrations in the crystal  $N_{dc1} < N_{d0} < N_{dc2}$ , the point defects interact nonlinearly to create an antisymmetric cluster (formula (14)). Owing to the self-consistent electron-deformation coupling, the electron density becomes redistributed, and a triple electric layer emerges. In Fig. 1, the coordinate dependences of the electrostatic potential for various average values of the conduction electron concentration are shown. As the concentration of electrons grows from  $2.6 \times 10^{17}$  to  $1.6 \times 10^{19} \text{ cm}^{-3}$ , the region of the barrier structure becomes more abrupt. Accordingly, the width of the junction layer decreases from 120 to 80 Å (Fig. 2). If  $\theta_d > 0$ , a double  $n - n^+ - n$  junction is formed, otherwise, if  $\theta_d < 0$ , an  $n^+ - n - n^+$

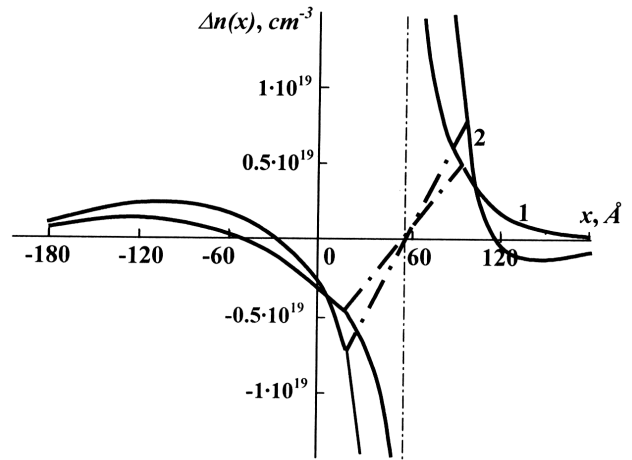


Fig. 2. Spatial redistribution of conduction electrons for various values of their average concentration  $n_0 = 2.6 \times 10^{17}$  (1) and  $1.6 \times 10^{19} \text{ cm}^{-3}$  (2). Dash-dotted lines correspond to the dependence  $x = a^{-1/2} \sinh^{-1} B$ .  $N_{d0} = 0.5 \times N_{dc}(1 + (l_0/l_d)^2)$

one. This phenomenon is associated with the growth of the conduction electron concentration in that crystal region where the point defects — vacancies — become accumulated ( $\theta_d < 0$ ). On the contrary, in the region, where interstitial atoms are accumulated ( $\theta_d > 0$ ), there is a lack of electrons ( $\Delta n(x) < 0$ ). The divergence of the solution at  $x \rightarrow a^{-1/2} \sinh^{-1} -B$  is caused by the neglect of the higher-order derivatives in the expansion series of the interatomic interaction operators [2]. If one does take those higher-order derivatives into account, then, in the vicinity of the plane  $x = a^{-1/2} \sinh^{-1} B$ , there will be a transition region (dash-dotted lines in Fig. 2) in the antisymmetric deformation well with a finite amplitude of the electron redistribution  $\Delta n(x)$ . The width of the internal electric layer depends on both the electron population  $\bar{n}$  of the conduction band and the defect concentration  $N_{d0}$ . As the concentration of defects increases, the width of the internal region increases too. Within the range  $N_{dc2} < N_{d0} < N_{dc}$  of the point defect concentration, the picture does not change qualitatively. In this case, a symmetric potential (Fig. 3) and, correspondingly, a symmetric triple electric layer appear. If the electron concentration grows from  $5 \times 10^{17}$  to  $3.2 \times 10^{19} \text{ cm}^{-3}$ , the height of the electric barrier increases by 0.4 V. The width of the electrostatic barrier region and the barrier height (Fig. 3) are characterized by the parameter  $\kappa = g_S(n)/\sqrt{a(N_{d0}, n)}$ . The growth of the electron concentration is accompanied by the growth of the electric barrier height. In Fig. 4, the redistribution

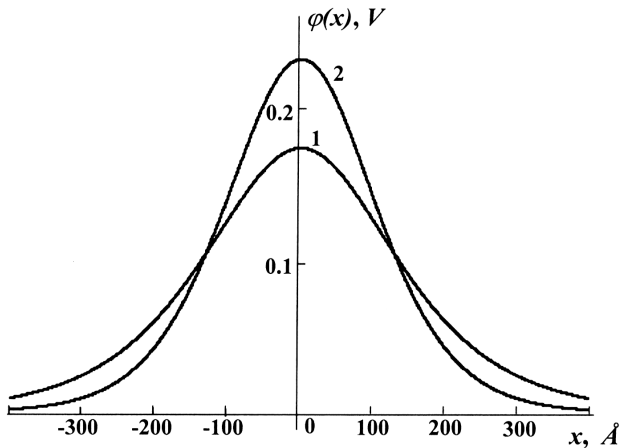


Fig. 3. Coordinate dependences of the electrostatic potential for various average values of the electron concentration  $n_0 = 5 \times 10^{17}$  (1) and  $3.2 \times 10^{19} \text{ cm}^{-3}$  (2).  $N_{d0} = N_{dc}(1 - \alpha^2/(9\beta))$

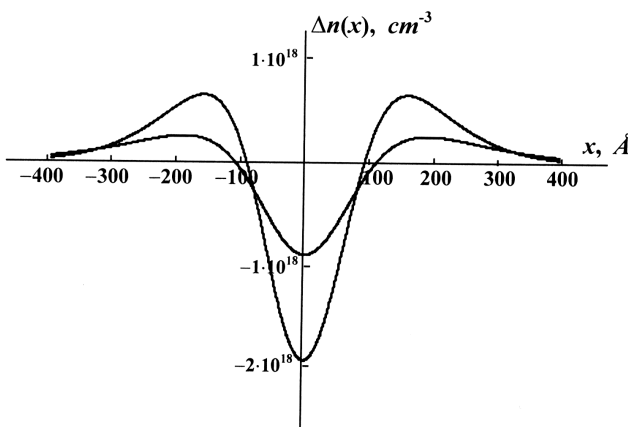


Fig. 4. Spatial redistribution of conduction electrons for various values of their average concentration  $n_0 = 5 \times 10^{17}$  (1) and  $3.2 \times 10^{19} \text{ cm}^{-3}$  (2).  $N_{d0} = N_{dc}(1 - \alpha^2/(9\beta))$

parameter of the electronic density is depicted for various average values of the current carrier concentration. The increase of the conduction band population leads to a reduction of the internal electric layer of the double  $n^+ - n$  junction.

If the concentration of defects grows further,  $N_{d0} > N_{dc}$ , the electron density becomes redistributed periodically in space (Fig. 5), and the periodic electrostatic potential emerges (Fig. 6). The origin of this phenomenon is the formation of strongly anharmonic periodic DD structures. In this case, there appear  $n - n^+$  junctions in the crystal, which are connected in series. The spatial period of the  $n - n^+$ -junction structure and the dimension of every electric layer are governed by the

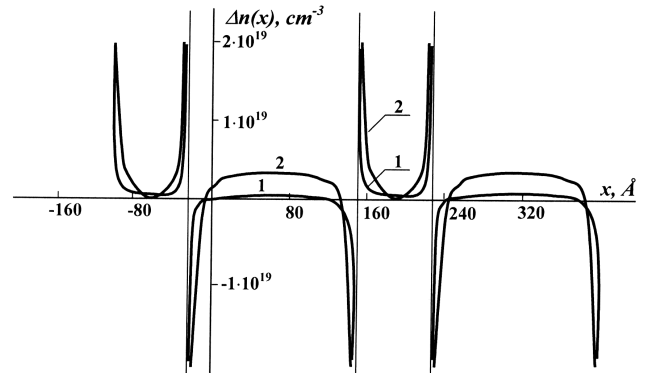


Fig. 5. Spatial redistribution of conduction electrons for various values of their average concentration  $n_0 = 2.6 \times 10^{18}$  (1) and  $1.0 \times 10^{20} \text{ cm}^{-3}$  (2).  $N_{d0} = 2N_{dc}$

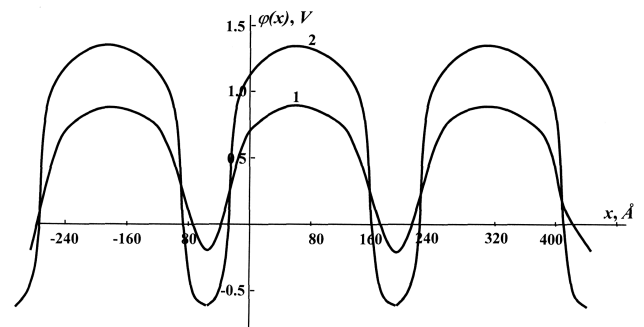


Fig. 6. Coordinate dependences of the electrostatic potential for various average values of the electron concentration  $n_0 = 2.6 \times 10^{18}$  (1) and  $1.0 \times 10^{20} \text{ cm}^{-3}$  (2).  $N_{d0} = 2N_{dc}$

concentration of defects, the deformation potential constant, the electron concentration, and the elastic constants. If the concentration of conduction electrons increases, the periodic electrostatic barrier structure obtains a more pronounced character. The increase of the point defect concentration causes a reduction of the spatial period of the  $n - n^+$ -junction structure.

#### 4. Conclusions

1. The criterion for the  $n - n^+$  junctions to appear in the crystals with self-assembled defect-deformation structures is the magnitude of the defect concentration  $N_{d0}$ . At  $N_{d0} < N_{dc1} = 3 \times 10^{18} \text{ cm}^{-3}$ , no  $n - n^+$  junctions appear in the crystal. At  $N_{d0} > N_{dc} = 10^{20} \text{ cm}^{-3}$ , the periodically arranged and connected in series  $n - n^+$  junctions are formed.

2. In the defect concentration range  $N_{dc1} < N_{d0} < N_{dc}$ , double junctions are formed.

3. It has been found that the height of the electrostatic barrier at a symmetric or antisymmetric nanocluster depends on the ratio between the nanocluster size  $1/\sqrt{\tilde{a}}$  and the effective screening radius of the electron-deformation interaction  $g_S^{-1}$ .

4. It has been shown that, as the defect concentration  $N_{d0}$  increases, the width of the internal electric layer of the double  $n - n^+ - n$  junction grows, and the spatial period of the  $n - n^+$  junctions connected in series diminishes. The growth of the deformation potential constant and the conduction electron constant is accompanied by a reduction of both the width of the internal electric layer of the double  $n - n^+ - n$  junction and the period of the  $n - n^+$  junctions connected in series. The presence of  $n - n^+$  junctions should manifest itself in experiments, while measuring the volt-ampere and volt-farad characteristics of the crystals with self-assembled nanoclusters.

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ВИНИКНЕННЯ  $n - n^+$ -ПЕРЕХОДІВ  
У КРИСТАЛАХ З САМООРГАНІЗОВАНИМИ  
ДЕФЕКТНО-ДЕФОРМАЦІЙНИМИ СТРУКТУРАМИ

*Р.М. Пелещак, О.В. Кузык*

Р е з ю м е

Побудовано теорію утворення подвійних та періодичних  $n - n^+$ -переходів у кристалах із самоорганізованими дефектно-деформаційними структурами.