

Role of Acoustoelectric Interaction in the Formation of Nanoscale Periodic Structures of Adsorbed Atoms

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Abstract—The role of acoustoelectric effects in the formation of nanoscale structures of adatoms, resulting from the self-consistent interaction of adatoms with a surface acoustic wave and the electronic subsystem, is studied for the case of charged and uncharged adatoms. It is shown that an increase in the doping level of a semiconductor with donor impurities at a fixed average adatom concentration results in an increase in the critical temperature below which self-organization processes occur.

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1. INTRODUCTION

Recently, the subject of intensive studies is the fabrication of semiconductor structures with self-assembled nanoclusters by molecular-beam epitaxy [1, 2] and ion-implantation [3, 4] methods, and the controllability of their physical properties. To optimize the technological processes and predictable control of the physical parameters of semiconductor structures with nanoclusters, information on the initial stage of the formation (nucleation) of periodic nanostructures of adatoms and implanted impurities is important.

In [5], nonlinear diffusion deformation theory of the self-assembly of nanoclusters of implanted impurities in semiconductor bulk, which takes into account the elastic interaction of implanted impurities with each other and with matrix atoms, was developed. An impurity appearing in the matrix causes a change in its volume and energy, and the initial deformation fluctuation predetermines the appearance of deformation-induced flows of implanted impurities under certain conditions.

As a result, forces proportional to the concentration and deformation gradients which additionally deform the matrix appear in the nonuniform deformation–concentration field. These forces cause an increase in the initial fluctuation and lead to the self-assembly of impurity clusters.

In [6], a theory of the spontaneous nucleation of surface nanoscale lattice, which is caused by instability in the system of neutral adatoms interacting with the self-consistent surface acoustic wave (SAW), was developed. Within this theory, the conditions of the formation of nanoclusters on a solid surface were determined and the nanoscale lattice constants were

determined as functions of the adatom concentration and temperature. In addition to instability in the system of adatoms, appearing due to their interaction via the mechanical deformation field [6], an additional instability caused by the self-consistent electron–deformation interaction appears [7].

Periodic deformation appearing on a semiconductor surface leads to modulation of the bottom of the conduction band, hence, to electron-density modulation. As a result, a nonuniform electric field arises, which cause nonuniform displacements of lattice sites, hence, a change in the SAW amplitude. During defect self-organization in semiconductor structures, there is an important question: are adatoms neutral or ionized donors (acceptors). In the latter case, the interaction of ionized adatoms with an internal electric field induced due to their periodic spatially inhomogeneous redistribution should also be taken into account.

In this work, the effect of the interaction of the SAW with the electronic subsystem on the conditions of the formation of periodic nanoscale adatom structures and their periods is studied.

2. DEFORMATION ON A SEMICONDUCTOR SURFACE TAKING INTO ACCOUNT ACOUSTOELECTRIC INTERACTION

The equation for the displacement vector u of an elastic medium is given by [6, 8]

$$\frac{\partial^2 \mathbf{u}}{\partial t^2} = c_l^2 \Delta \mathbf{u} + (c_l^2 - c_t^2) \text{grad}(\text{div} \mathbf{u}), \quad (1)$$

where c_l and c_t are the longitudinal and transverse speeds of sound, respectively.

Let the semiconductor surface coincide with the $z = 0$ plane (the z axis is directed to the crystal depth). Let us assume that a surface perturbation of the elastic medium arises along the x axis, which we set as a static SAW rapidly damping to the semiconductor depth and having an amplitude increasing with time [6],

$$u_x = -iqR \exp(iqx + \lambda t - k_l z) - ik_l Q \exp(iqx + \lambda t - k_l z), \quad (2)$$

$$u_z = k_l R \exp(iqx + \lambda t - k_l z) + qQ \exp(iqx + \lambda t - k_l z), \quad (3)$$

where $k_{l,t}^2 = q^2 + \frac{\lambda^2}{c_{l,t}^2}$, λ is the defect–deformation instability increment [6], R and Q are the SAW amplitudes.

Then the deformation ε on the semiconductor surface ($z = 0$) is written as

$$\varepsilon = \frac{\partial u_x}{\partial x} + \frac{\partial u_z}{\partial z} = -\frac{\lambda^2}{c_l^2} R \exp(iqx + \lambda t). \quad (4)$$

Let us consider two cases:

(i) a doped n -type semiconductor containing impurities (ionized donors), free electrons, and adatoms which are also ionized donors; and

(ii) a doped n -type semiconductor containing impurities (ionized donors), free electrons, and neutral adatoms.

For these cases, the electrical-neutrality conditions

$$n_0 = N_d^+ + N_0, \quad (5)$$

$$n_0 = N_d, \quad (6)$$

respectively, should be satisfied, where N_d , n_0 , and N_0 are the surface concentration of ionized donors, and spatially uniform values of the surface concentrations of electrons and adatoms, respectively.

Periodic surface deformation results in the spatially inhomogeneous redistribution of adatoms $N(x)$, modulation of the bottom of the conduction band, hence, redistributions of the conduction-electron density $n(x)$ and the electrostatic potential $\varphi(x)$,

$$N(x) = N_0 + N_1(x) = N_0 + N_1(q) \exp(iqx + \lambda t), \quad (7)$$

$$n(x) = n_0 + n_1(x) = n_0 + n_1(q) \exp(iqx + \lambda t), \quad (8)$$

$$\varphi(x) = \varphi(q) \exp(iqx + \lambda t), \quad (9)$$

where $N_1(q)$, $n_1(q)$, $\varphi(q)$ are the amplitudes of the corresponding periodic perturbations.

As a result of spatial redistribution of the electric charge on the semiconductor surface along the x axis, a nonuniform electric field $E_s(x)$ is induced, which causes the nonuniform displacement of lattice sites,

hence, the appearance of additional mechanical deformation σ_{xx}^{el} ,

$$\sigma_{xx}^{el} = \frac{e}{a} \frac{\partial E_s(x)}{\partial x} = -\frac{e}{a} \frac{\partial^2 \varphi(x)}{\partial x^2}, \quad (10)$$

where a is the lattice period. Then the components of the tensor of the deformation caused by acoustoelectric interaction are written as

$$\varepsilon_{xx}^{el} = -\frac{e}{aE} \frac{\partial^2 \varphi(x)}{\partial x^2}, \quad \varepsilon_{zz}^{el} = \frac{\nu e}{aE} \frac{\partial^2 \varphi(x)}{\partial x^2}, \quad (11)$$

where E and ν are Young's modulus and the Poisson ratio, respectively. The Poisson equation, taking into account Eqs. (5)–(9) takes the form

$$-q^2 \varphi(q) = \frac{e}{\varepsilon_0 \tilde{\varepsilon} a} (n_1(q) - N_1(q)), \quad (12a)$$

in the case of charged adatoms and

$$-q^2 \varphi(q) = \frac{e}{\varepsilon_0 \tilde{\varepsilon} a} n_1(q), \quad (12b)$$

in the case of neutral adatoms, where ε_0 and $\tilde{\varepsilon}$ are the dielectric constant and medium permittivity, respectively.

Then deformation on the semiconductor surface, caused by acoustoelectric interaction is written as

$$\varepsilon^{el} = \varepsilon_{xx}^{el} + \varepsilon_{zz}^{el} = -\frac{e^2(1-\nu)}{\varepsilon_0 \tilde{\varepsilon} a^2 E} (n_1(q) - N_1(q)) \exp(iqx + \lambda t), \quad (13a)$$

$$\varepsilon^{el} = -\frac{e^2(1-\nu)}{\varepsilon_0 \tilde{\varepsilon} a^2 E} n_1(q) \exp(iqx + \lambda t). \quad (13b)$$

As can be seen from formulas (13a) and (13b), electron–deformation interaction leads to additional lattice compression in regions of electron accumulation and, on the contrary, additional tension in regions with electron densities lower than the average value.

3. FORMATION OF THE PERIODIC STRUCTURE OF CHARGED ADATOMS

The equation for the concentration of charged adatoms, taking into account acoustoelectric interaction, is written as

$$\frac{\partial N}{\partial t} = D_d \frac{\partial^2 N}{\partial x^2} + \frac{\partial}{\partial x} \left(\mu_d N \frac{\partial \varphi}{\partial x} \right) - D_d \frac{\theta_d}{kT} \frac{\partial}{\partial x} \left(N \frac{\partial}{\partial x} \left(\varepsilon + \varepsilon^{el} + l_d^2 \frac{\partial^2 (\varepsilon + \varepsilon^{el})}{\partial x^2} \right) \right), \quad (14)$$

where D_d and μ_b are the surface diffusion coefficient and adatom mobility, which are related by the Einstein relation $\mu_d = D_d \frac{e}{k_B T}$ (k_B is the Boltzmann constant and T is the temperature), θ_d is the deformation potential,

and l_d is the characteristic length of the interaction of adatoms with lattice atoms. The second term accounts for the interaction of adatoms with an electric field induced due to the spatially inhomogeneous redistribution of electric charge; the third term expresses the interaction of adatoms with the deformation field, taking into account nonlocal interaction [6].

Taking into account Eqs. (4), (7)–(9), (13), in the approximation $N_1 \ll N_0$, we write Eq. (14) in the form

$$\begin{aligned} \lambda N_1(q) = & -D_d q^2 N_1(q) + \frac{D_d N_0 \Phi}{kT} (n_1(1) - N_1(q)) \\ & - \frac{D_d N_0 \theta_d}{kT} \left(\frac{\lambda^2}{c_l^2} R q^2 (1 - q^2 l_d^2) \right) \\ & + \frac{\Phi q^2 (1 - q^2 l_d^2)}{2a\rho c_l^2 \beta (3 - 4\beta)} (n_1(q) - N_1(q)), \end{aligned} \quad (15)$$

where $\Phi = \frac{e^2}{\epsilon_0 \tilde{\epsilon} a}$, ρ is the medium density, and $\beta = \frac{c_l^2}{c_i^2}$.

The electric-current density of electrons is given by

$$j = n\mu_n \frac{d\chi}{dx}, \quad (16)$$

where μ_n is the electron mobility. The electrochemical potential χ is given by

$$\chi(x) = k_B T \ln \frac{n(x)}{N_i} - e\phi(x) + a_c(\epsilon(x) + \epsilon^{el}(x)), \quad (17)$$

where $N_i = 2 \left(\frac{2\pi m k T}{h^2} \right)^{3/2}$ is the effective density of states, a_c is the constant of the hydrostatic deformation potential of the conduction band. Then the continuity equation taking into account Eqs. (16), (17) can be written as

$$\begin{aligned} e \frac{\partial n}{\partial t} = & k_B T \mu_n \frac{\partial}{\partial x} \left(n \frac{\partial}{\partial x} \ln \frac{n}{N_i} \right) - e \mu_n \frac{\partial}{\partial x} \left(n \frac{\partial \phi}{\partial x} \right) \\ & + a_c \mu_n \frac{\partial}{\partial x} \left(n \frac{\partial}{\partial x} (\epsilon + \epsilon^{el}) \right). \end{aligned} \quad (18)$$

Taking into account Eqs. (4), (7)–(9), (13), we write Eq. (18) in the form

$$\begin{aligned} n_1(q)(e\lambda + k_B T \mu_n q^2 + n_0 \mu_n \Phi (1 + q^2 r^2)) \\ = N_1(q) n_0 \mu_n \Phi (1 + q^2 r^2) + a_c n_0 \mu_n q^2 \frac{\lambda^2}{c_l^2} R, \end{aligned} \quad (19)$$

where $r^2 = -\frac{a_c}{2a\rho c_l^2 \beta (3 - 4\beta)}$. Here it is taken into account that $a_c < 0$.

Having solved system of equations (15) and (19), we obtain expressions for the amplitudes of the surface concentrations of adatoms $N_1(q)$ and conduction electrons $n_1(q)$.

The spatially inhomogeneous distribution of adatoms modulates the surface energy $F(x)$, which gives rise to the lateral mechanical stress $\sigma_{xz} = \frac{\partial F(N(x))}{\partial x}$ which is compensated by the shear stress in a medium [6]. The boundary condition expressing the balance of lateral stresses has the form

$$\frac{E}{1 + \nu} \left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} \right)_{z=0} = \frac{\partial F(N(x))}{\partial x} = \frac{\partial F}{\partial N} \frac{\partial N_1(x)}{\partial x}. \quad (20)$$

Furthermore, the interaction of adatoms with semiconductor atoms on the surface results in normal mechanical stress; the corresponding boundary condition is written as

$$\begin{aligned} \frac{E}{1 + \nu} \left(\frac{\partial u_z}{\partial z} + \epsilon_{zz}^{el} + \frac{\nu}{1 - 2\nu} \left(\frac{\partial u_x}{\partial x} + \epsilon_{xx}^{el} \right) \right)_{z=0} \\ = \frac{\theta_d}{a} N_1(x). \end{aligned} \quad (21)$$

Thus, we obtain the system of linear homogeneous equations (20) and (21) with respect to the amplitudes R and Q . Then from the solution nontriviality condition, we can obtain the dispersion dependences $\lambda(q)$.

The dependences $\lambda(q)$ were calculated for the semiconductor GaAs at the following parameters: $ld = 2.9$ nm, $a = 0.565$ nm, $c_l = 4400$ m/s, $c_i = 2475$ m/s, $\rho = 5320$ kg/m³, $a_c = -7.17$ eV, $T = 300$ K, $D_d = 5 \times 10^{-9}$ cm²/s, $\theta_d = 10$ eV, $\tilde{\epsilon} = 12$, and $\mu_n = 8 \times 10^3$ cm²/(V s).

Figure 1 shows the calculated dependence of the defect–deformation instability increment on the wave-vector magnitude at various concentrations of ionized donors N_d and various average adatom concentrations N_0 . This dependence has a maximum which shifts to higher wave-vector magnitudes with increasing concentrations of ionized donors (free electrons). The value q_{\max} at which the defect–deformation instability increment has a maximum defines

the dominant structure period $d = \frac{2\pi}{q_{\max}}$ (Fig. 2). As the concentration of ionized donors increases, the acoustoelectric effects lead to an increase in the defect–deformation instability increment. Thus, the formation of nanoscale periodic structures should occur more rapidly in semiconductors with a high donor-impurity doping level. The role of acoustoelectric effects in the formation of periodic adatom lattices is more significant at lower adatom concentrations (Fig. 1). For example, for the average adatom concentration $N_0 = 3 \times 10^{12}$ cm⁻², the defect–deformation

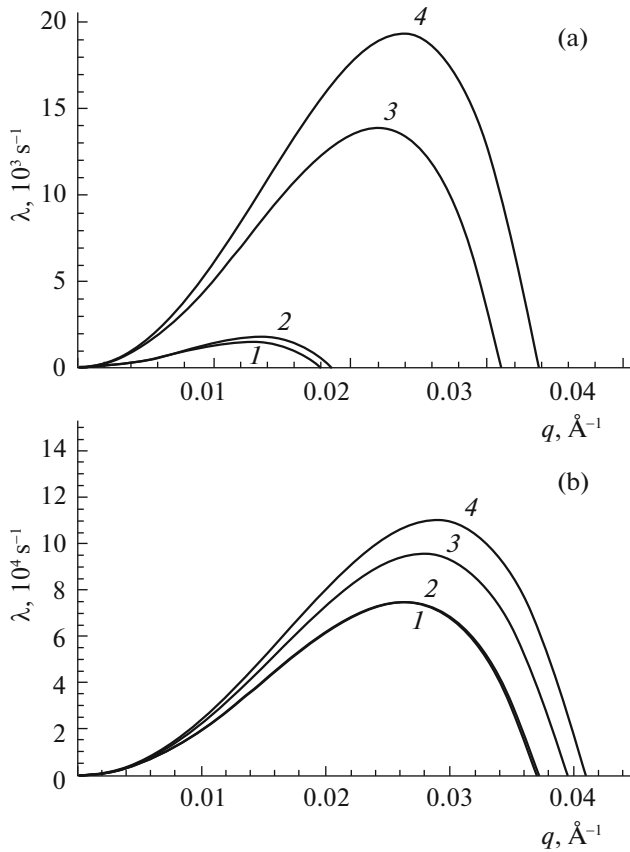


Fig. 1. Dependence of the defect–deformation instability increment on the wave-vector magnitude at various ionized-donor concentrations $N_d = (1) 10^9$, $(2) 10^{11}$, $(3) 10^{13}$, and $(4) 10^{14} \text{ cm}^{-2}$; $N_0 = (a) 3 \times 10^{12}$ and $(b) 8 \times 10^{12} \text{ cm}^{-2}$.

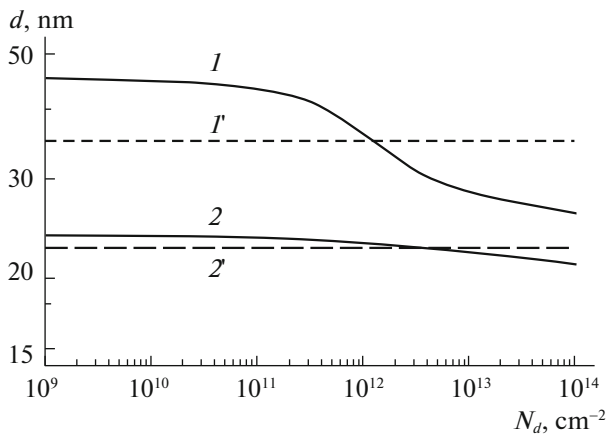


Fig. 2. Dependence of the period of the surface defect–deformation structure on the concentration of ionized donors at various average adatom concentrations: at the adatom concentration $N_0 = 3 \times 10^{12} \text{ cm}^{-2}$ (1) with and $(1')$ without electron–deformation interaction taken into account; at the adatom concentration $N_0 = 8 \times 10^{12} \text{ cm}^{-2}$ (2) with and $(2')$ without electron–deformation interaction taken into account.

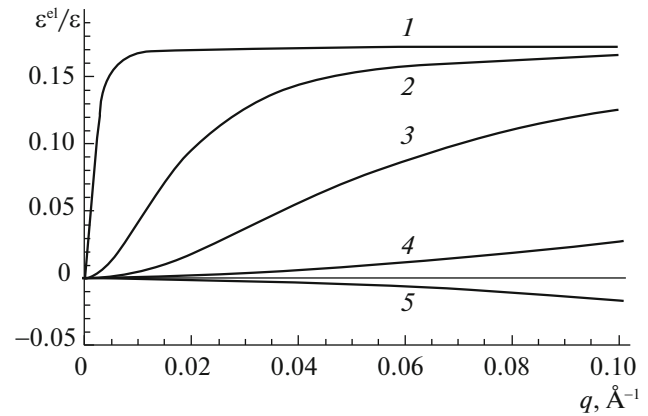


Fig. 3. Dependence of the fraction of the electron-deformation component on the wave-vector magnitude at the various ionized donor concentrations $N_d = (1) 10^8$, $(2) 10^{10}$, $(3) 10^{11}$, $(4) 10^{12}$, and $(5) 10^{14} \text{ cm}^{-2}$.

instability increment increases by a factor of ~ 13 as the donor concentration increases from 10^9 to 10^{14} cm^{-2} (Fig. 1a), whereas this factor is only 1.5 at $N_0 = 8 \times 10^{12} \text{ cm}^{-2}$ (Fig. 1b).

The same systematic feature is also observed for the period of the dominant defect–deformation lattice (Fig. 2). For the average adatom concentration $N_0 = 3 \times 10^{12} \text{ cm}^{-2}$, the defect–deformation structure period steadily decreases from 45 to 25 nm as the donor concentration increases from 10^9 to 10^{14} cm^{-2} ; at $N_0 = 8 \times 10^{12} \text{ cm}^{-2}$, it decreases from 23 to 21 nm. Therewith, approximately to a donor concentration lower than the average adatom concentration, electron–deformation effects lead to an increase in the adatom lattice period; at larger donor concentrations, these effects lead to a decrease in the period. This results from the fact that the amplitude of spatial perturbations of adatoms at low donor concentrations is higher than the corresponding amplitude for conduction electrons ($N_1(q) > n_1(q)$), and the electronic–deformation component ϵ^{el} (formula (13a)) is predominantly controlled by the concentration of positively charged adatoms. In this case, the sign of the electronic component at each surface point is identical to the sign of the mechanical deformation appearing due to the presence of adatoms (Fig. 3, curves 1–4). At donor concentrations higher than the average adatom concentration, the electronic –deformation component is controlled by the spatial distribution of conduction electrons. In this case, $n_1(q) > N_1(q)$ and the electronic–deformation component is opposite to the mechanical deformation appearing due to the presence of adatoms (Fig. 3, curve 5).

The formation of self-assembled periodic defect–deformation structures is possible only if the adatom concentration exceeds a certain critical value N_c . Figure 4 shows the dependence of the critical adatom

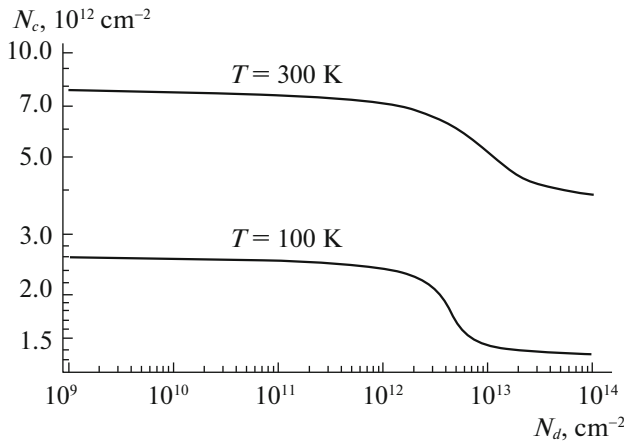


Fig. 4. Dependence of the critical adatom concentration on the ionized-donor concentration.

concentration on the doping level of a semiconductor with donor impurities at various temperatures. The results obtained show that an increase in the ionized-donor concentration (conduction electron density) leads to a decrease in the crucial adatom concentration at which the formation of the nanoscale adatom lattice is possible. More precisely, at $T = 100$ K, the critical value N_c decreases from 2.6×10^{12} to $1.35 \times 10^{12} \text{ cm}^{-2}$, as the ionized-donor concentration varies from 10^9 to 10^{14} cm^{-2} ; at $T = 300$ K, N_c decreases from 7.8×10^{12} to $3.91 \times 10^{12} \text{ cm}^{-2}$. As seen in Fig. 4, adatom self-organization processes occur more efficiently at lower temperatures. This is identical to the results obtained in [6], where it is shown that the defect–deformation lattice can be formed only at temperatures lower than a certain critical value. An increase in semiconductor doping level with donor impurities makes it possible to increase the temperature at which nanostructure self-assembly processes are possible.

4. FORMATION OF THE STRUCTURE OF NEUTRAL ADATOMS

In this case, Eqs. (15) and (19), taking into account Eq. (13b), can be written as

$$(\lambda + D_d q^2) N_1(q) = - \frac{D_d N_0 \theta_d q^2 (1 - q^2 l_d^2)}{kT} \times \left(\frac{\lambda^2}{c_l^2} R + \frac{\Phi}{2\alpha p c_l^2 \beta (3 - 4\beta)} n_1(q) \right), \quad (22)$$

$$n_1(q) (e\lambda + k_B T \mu_n q^2 + n_0 \mu_n \Phi (1 + q^2 r^2)) = a_c n_0 \mu_n q^2 \frac{\lambda^2}{c_l^2} R. \quad (23)$$

In the limit $n_0 \rightarrow 0$, Eq. (22) is identical to the corresponding equation in [6]. As the surface density of free electrons increases, the amplitude $n_1(q)$ steadily increases, asymptotically approaching the value

$$\lim_{n_0 \rightarrow \infty} n_1(q) = \frac{a_c q^2 \frac{\lambda^2}{c_l^2} R}{\Phi (1 + q^2 r^2)} \approx \frac{a_c q^2 \frac{\lambda^2}{c_l^2} R}{\Phi}.$$

Then the ratio of the electronic-deformation component to the mechanical deformation appearing due to the spatial redistribution of adatoms on the semiconductor surface is independent of the electron density and is given by

$$\frac{\varepsilon^{el}}{\varepsilon} = \frac{(1 - \nu) a_c q^2}{a E} = \frac{a_c q^2}{2\alpha p c_l^2 \beta (3 - 4\beta)}. \quad (24)$$

Thus, the contribution of the electronic-deformation component increases with the wave-vector magnitude according to parabolic law and cannot exceed 2% (at $q = 1 \text{ nm}^{-1}$) of the mechanical deformation. At lower surface electron densities, this value is even lower. Thus, it can be concluded that the role electron–deformation effects is insignificant in the case of unionized adatoms.

The proposed model does not take into account the surface modulation of donors. Such an approximation is valid if the deformation potential of dopants is insignificant in comparison with the deformation potential of adatoms.

5. CONCLUSIONS

(i) The role of acoustoelectric effects in the formation of nanoscale adatom structures, resulting from the self-consistent interaction of adatoms with the surface acoustic wave and the electronic subsystem in the case of charged and uncharged adsorbed atoms was studied.

(ii) It was shown that, in the case of charged adatoms in semiconductor GaAs, an increase in the donor dopant concentration results in a decrease in the critical adatom concentration at which the formation of self-assembled nanostructures is possible or an increase in the semiconductor doping level with donor impurities (an increase in the free electron density) at a fixed average adatom concentration results in an increase in the critical temperature below which self-assembly processes occur.

(iii) It was found that an increase in the donor dopant concentration in the case of charged adatoms in semiconductor GaAs leads to a decrease in the period of self-assembled surface nanostructures of adatoms.

(iv) It was shown that acoustoelectric interaction causes a change in the inhomogeneous deformation resulting from the spatial redistribution of adatoms. It

was found that, depending on the semiconductor doping level with donor impurities, the strain can vary up to 17% in the case of ionized adatoms and only up to 2% in the case of uncharged adatoms.

REFERENCES

1. N. N. Ledentsov, V. M. Ustinov, V. A. Shchukin, P. S. Kop'ev, Zh. I. Alferov, and D. Bimberg, *Semiconductors* **32**, 343 (1998).
2. I. P. Ipatova, V. G. Malyskin, and A. A. Maradudin, *Phys. Rev. B* **57**, 968 (1998).
3. I. Yamada, J. Matsuo, and N. Tojoda, *Nucl. Instrum Methods Phys. Res. B* **206**, 820 (2003).
4. A. V. Boryakov, D. E. Nikolichev, D. I. Tetelbaum, A. I. Belov, A. V. Ershov, and A. N. Mikhailov, *Phys. Solid State* **54**, 394 (2012).
5. R. M. Peleshchak, O. V. Kuzyk, and O. O. Dan'kiv, *J. Phys. Studies* **17**, 2601 (2013).
6. V. I. Emel'yanov and K. I. Eremin, *JETP Lett.* **75**, 98 (2002).
7. I. V. Stasyuk and R. M. Peleshchak, *Ukr. J. Phys.* **36**, 1744 (1991).
8. L. D. Landau and E. M. Lifshitz, *Course of Theoretical Physics*, Vol. 7: *Theory of Elasticity* (Nauka, Moscow, 1965; Pergamon Press, New York, 1986).

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