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ELASTIC STRAINS IN SiGe HETEROSTRUCTURES WITH NON-UNIFORM QUANTUM DOTS

Elastic strain distributions in SiGe heterostructures with quantum dots have been simulated with the use of the finite element method. The effect of a non-uniform germanium distribution in the nanoislands on the spatial dependence and the magnitude of elastic fields was studied. It is shown that quantum dots with a uniform component content are more strained in comparison with non-uniform nanoislands.

Keywords: Stranski–Krastanov growth mode, Green's functions, finite element method, wetting layer, stress tensor, elastic moduli tensor, rigid boundary conditions, node, Galerkin method.

1. Introduction

The unique electronic and optical properties of silicon–germanium heterostructures with self-organized quantum dots (nanoislands) create a basis for their practical application as promising materials to modern nano- and optoelectronics [1]. In particular, a high absorption factor of those heterostructures in the range of energies lower than the germanium energy gap width is successfully used in the manufacture of infra-red radiation detectors of a new generation [2]. Moreover, silicon–germanium structures can serve as active elements in solar batteries [3] and light emitting [4] and spintronic [5] devices.

The properties of silicon heterostructures $Si_{1-x}Ge_x$ with quantum dots, where x is the germanium content in the compound, obtained following the Stranski–Krastanov growth mode are closely connected with elastic deformations and accompanying mechanical stress fields in the structures. It is the elastic fields arising owing to the mismatch between the material lattices that play a crucial role in the growing of a heterostructure, being responsible for a spatial ordering of nanoislands and their shape [6]. Moreover, elastic strains substantially affect the band structure (the confinement-potential for charge carriers) of crystals, the mobility and the effective masses of electrons and holes in them, and, hence, change the properties of heterostructures on the whole [7]. Therefore, an important task of the physics and the technology of nanodimensional semiconducting structures consists in developing the methods for the determination of and the control over elastic strain fields, as well as their manipulation by means of varying the physical parameters of heterostructures.

Experimental researches of mechanical stresses in low-dimensional heterostructures are based on the Raman scattering technique [8, 9]. In particular, this method enables the peculiarities in a crystal structure of strained germanium nanoislands in the silicon matrix [10] or their morphology [11] to be determined. However, the analysis of Raman spectra allows only the averaged values of strains to be estimated and provides no information concerning their distribution in the islands and near to them. Taking all the above into account, the methods of computer simulation turn out an effective tool to research nanosystems, in particular, silicon–germanium heterostructures.

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For today, there are plenty of works devoted to the study of elastic strain fields and their influence on the properties of $Si_{1-x}Ge_x$ heterostructures with quantum dots [12–14]. There are a number of approaches to calculate the elastically deformed state of structures with nanoislands; they use the molecular dynamics, Green's function, or finite element methods [15–17]. The shortcoming of the former consists in a considerable computation time even if objects with small volume are calculated. The Green's function method is used mostly if the structures are analyzed in the approximation of infinite or semiinfinite substrate; however, it cannot be always applied to confined systems. The most widespread is the method of finite elements, which allows the calculations to be carried out for objects with complicated geometry and does not require considerable computational resources.

In the majority of the known works, where the heterostructure properties induced by elastic fields are studied, the obtained results are analyzed making the assumption that the component content in nanoislands is uniform. However, in the course of high-temperature epitaxy of germanium onto a silicon substrate, the components become partially mixed, so that their contents change over the quantum dot volume. As was shown in work [18], the redistribution of the silicon and germanium concentrations in nanoislands results in a decrease of the energy of the system, and this redistribution therefore turns out to be energetically beneficial. The corresponding distribution of germanium (silicon) is related to the shape of quantum dots and the content ratio between Si and Ge in them. Bearing in mind that the concentration gradient can be rather substantial, the account of a non-uniformity in the contents of island components is an important factor, while studying the properties that are governed by the electron structure of quantum dots, because this structure is sensitive to deformations in heterostructures.

In this work, we used the finite element method to calculate the strain fields in silicon heterostructures with germanium quantum dots. The calculations were carried out in the framework of the elastic continuum model. A comparative analysis of the results obtained for nanoislands with uniform and non-uniform germanium distributions over their volume was made. We also analyzed the influence of a component content non-uniformity on the band structure in $Si_{1-x}Ge_x$ quantum dots.

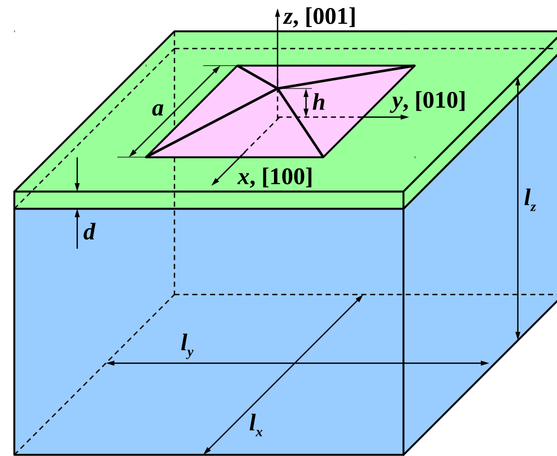

Fig. 1. Geometrical parameters of the studied SiGe heterostructure

2. Procedure for Calculating Strains in SiGe Heterostructures

We will consider self-organized germanium quantum dots on a silicon surface as a regular array of islands with identical dimensions. The typical period (the distance between neighbor nanoislands) in such heterostructures equals a few tens of nanometers. Therefore, while calculating elastic strains in the silicon substrate–germanium quantum dot system, let us confine the consideration to a single model cell that includes one quantum dot in the form of a regular square pyramid centered on a substrate with the transverse dimensions $l_x \times l_y$ and the thickness l_z (Fig. 1). Between the Si substrate and the germanium quantum dot, there is a wetting layer of Ge of the thickness d. The height and the base side length of the pyramid equal h and a, respectively. The origin of a coordinate system is fixed at the center of the pyramid base, and the x, y, and z axes are directed along the crystallographic directions [100], [010], and [001], respectively.

The strain fields in heterostructures with quantum dots will be studied in the elastic continuum approximation with the use of the standard equations of elasticity theory,

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0, \qquad (1)$$

$$\sigma_{ij} = C_{ijkl}\,[\varepsilon_{kl} - \varepsilon_{0kl}], \tag{2}$$

$$\varepsilon_{kl} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right), \tag{3}$$

where σ_{ij}, ε_{kl} and C_{ijkl} are the tensors of mechanical stresses, elastic strains, and elastic moduli, respectively; and u_k is the elastic displacement vector. The quantities ε_{0kl} in Eq. (2) stand for initial strains originated from a mismatch between the lattice parameters in the substrate and nanoisland materials (misfit strains),

$$\varepsilon_{0ij} = \frac{a_s - a_i}{a_s}\delta_{ij}, \tag{4}$$

where a_s and a_i are the lattice constants for the substrate and the quantum dot, respectively, and δ_{ij} is the Kronecker symbol. Since $a_s = 5.430$ Å for silicon and 5.646 Å for germanium, the absolute value of ε_{0ij} amounts to approximately 4%. In the calculations, the initial strain was considered to be nonzero only in the quantum dot. The subsequent structure relaxation resulted in the appearance of strains in the whole substrate as well.

Notice that the lattice mismatch is not the unique source of mechanical stresses. Since the heterostructures are grown up at epitaxial temperatures, their subsequent cooling down may invoke stresses stemming from the difference $\Delta\alpha$ between the thermal expansion coefficients. The corresponding strains $\varepsilon_{\rm TE}$ arisen in the structure can be estimated from the relation

$$\varepsilon_{\rm TE} = \Delta\alpha\Delta T, \tag{5}$$

where ΔT is the temperature change. We are interested in the strains that take place in heterostructures at room temperature, i.e. $\Delta T \simeq 500$ °C. Then, taking into account that $\Delta\alpha = 3.3 \times 10^{-6}$ °C^{-1} for the heteropair Si–Ge, we obtain the value $\varepsilon_{\rm TE} \approx 0.2\%$. Hence, the value of $\varepsilon_{\rm TE}$ is an order of magnitude less than the strains ε_{0ij}, and we will consider below only mechanical stress fields related to the lattice mismatch between the substrate and nanoisland materials.

Equations (1)–(3) have to be appended by boundary conditions for the unknown components of the displacement vector. In particular, in view of the periodic character of heterostructure, the normal components of the vector u_k were fixed at the opposite edges $x = \pm l_x/2$ and $y = \pm l_y/2$ of the model cell,

$$u_x\left(x = \pm\frac{l_x}{2}\right) = u_y\left(y = \pm\frac{l_y}{2}\right) = 0. \tag{6}$$

The thickness of the wetting layer near the quantum dot, where the strain fields are considered, is much narrower than the substrate thickness. Therefore, the following "rigid" boundary conditions are selected at the lower substrate edge $z = -l_z$:

$$u_i\,(z = -l_z) = 0, \quad i = x, y, z. \tag{7}$$

In addition, the absence of mechanical stresses is supposed at all external surfaces, including the open surfaces of germanium nanoislands and the silicon substrate.

The formulated problem has no analytical solution. Therefore, in this work, the elastic fields in silicon–germanium heterostructures are determined within the finite element method. The calculations were carriued out according to a Fortran program written by the author, in which the procedures of the Intel MKL mathematical library were used. The model cell containing a quantum dot on a silicon substrate was divided into a mesh of tetrahedral elements, each of them containing 10 nodes. Within every element, the unknown components of the elastic displacement vector were approximated by a linear combination of the so-called shape functions $\xi\,(x, y, z)$ [16],

$$u_k\,(x, y, z) = \sum_{i=1}^{10} \nu_{ik}\xi_i\,(x, y, z), \tag{8}$$

where ν_{ik} are the unknown coefficients equal to u_k-values at the mesh nodes. The application of the Galerkin method [19] allowed the differential equations (1)–(3) with the corresponding boundary conditions to be transformed into a system of algebraic equations for the unknown coefficients ν_{ik},

$$[K]\,[\nu] = [f], \tag{9}$$

where the components of the matrices $[K]$ and $[f]$ are determined by the relations

$$K = \int\limits_{Ve} B^T C B dV, \tag{10}$$

$$f = \int\limits_{Ve} B^T C \varepsilon_0 dV. \tag{11}$$

Integration in expressions (10) and (11) is carried out over the element volume V_e, the upper index T means the transposition operation, and B^T stands for the operator of the following form:

$$B^T = \begin{bmatrix} \frac{\partial \xi}{\partial x} & 0 & 0 & 0 & \frac{\partial \xi}{\partial z} & \frac{\partial \xi}{\partial y} \\ 0 & \frac{\partial \xi}{\partial y} & 0 & \frac{\partial \xi}{\partial z} & 0 & \frac{\partial \xi}{\partial x} \\ 0 & 0 & \frac{\partial \xi}{\partial z} & \frac{\partial \xi}{\partial y} & \frac{\partial \xi}{\partial x} & 0 \end{bmatrix}. \quad (12)$$

The coefficients ν_{ik} obtained from the solution of Eqs. (9) were used to calculate the components of the elastic displacement vector u_k. Then, with the use of relation (3), the strain tensor components were calculated.

3. Results and Their Discussion

Elastic strains in heterostructures were calculated for the following parameters of nanoislands: the base side length $a = 30$ nm, height $h = 4.5$ nm, and wetting layer thickness $d = 0.5$ nm. The dimensions of the model cell were chosen to equal the average distance between quantum dots in real structures, i.e. $l_x = l_y = 60$ nm. To exclude the influence of the lower substrate face, the dimension l_z was selected to be 10 times larger than the nanoisland height, $l_z = 10h = 45$ nm.

In the calculations connected with the non-uniform content of germanium in quantum dots, the distribution of the Ge concentration, whose profile is depicted in Fig. 2, was used. The exhibited dependence is similar to that obtained earlier in work [18] for pyramidal nanoislands. The maximum germanium content, $x \approx 1$, was observed near the island vertices, and its minimum, $x \approx 0.3$, in vicinities of the vertices near the base. The value of germanium content averaged over the whole quantum dot volume was about 0.7. Therefore, the data obtained for $Si_{1-x}Ge_x$ heterostructures with non-uniform nanoislands were compared with the results of calculations for islands with a uniform component content, $Si_{0.3}Ge_{0.7}$. The values of components of the tensor of elastic moduli for pure silicon, C_{ij}(Si), and germanium, C_{ij}(Ge), were taken from work [20]. For the compound $Si_{1-x}Ge_x$, the following linear approximation was used:

$$C_{ij}(Si_{1-x}Ge_x) = [C_{ij}(Ge) - C_{ij}(Si)]\, x + C_{ij}(Si). \quad (13)$$

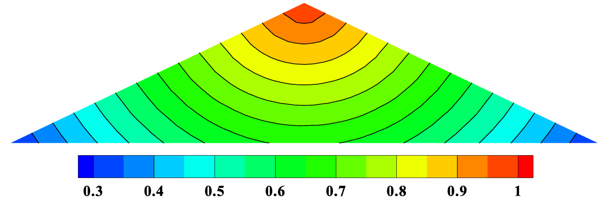

Fig. 2. Non-uniform distribution of the germanium content x in a pyramidal quantum dot $Si_{1-x}Ge_x$ used for the calculations of elastic fields

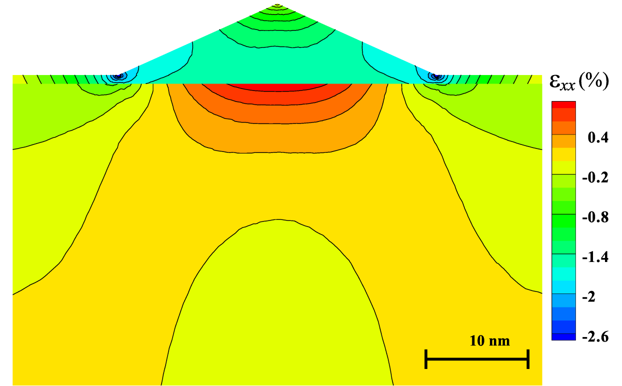

Fig. 3. Spatial distribution of the strain tensor component ε_{xx} in the xz-plane for a heterostructure with non-uniform $Si_{1-x}Ge_x$ nanoislands

In Fig. 3, the calculated distribution of the ε_{xx} component of the strain tensor in the heterostructure with a non-uniform nanoisland content is depicted. The ε_{xx} magnitude substantially varies in the quantum dot and near its base, so that high strain gradients arise in those heterostructure regions. One can see that the stretching strains prevail in the silicon substrate along the Si–$Si_{1-x}Ge_x$ heterojunction, with the maximum value $\varepsilon_{xx} = 0.6\%$ attaining near the island base. At the same time, the ε_{xx} component changes the sign in the quantum dot, and this section of the heterostructure undergoes compressive strains along the heterojunction with a maximum value of 2.5% near the base angles. The magnitude of compressive strains gradually decreases from the pyramid base to its vertex. The component ε_{yy} of the strain tensor has a similar dependence, and its distribution is not shown.

In the elastic deformation interval, the ratio between the longitudinal and transverse elongations is constant (the Poisson effect). Therefore, the strain

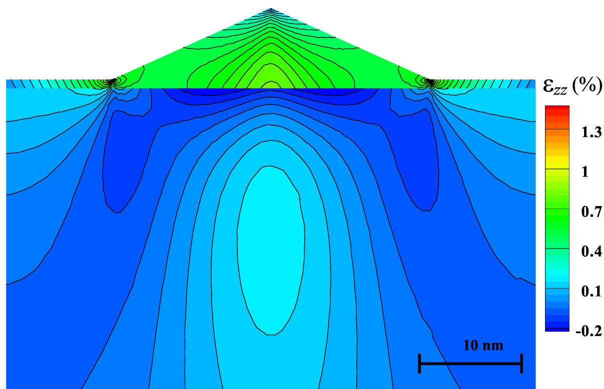

Fig. 4. The same as in Fig. 3, but for the strain tensor component ε_{zz}

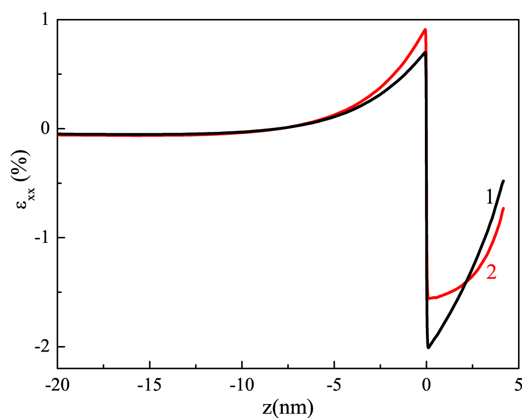

Fig. 5. Distributions of the strain tensor component ε_{xx} along the axis Oz in heterostructures with uniform (*1*) and non-uniform (*2*) nanoislands

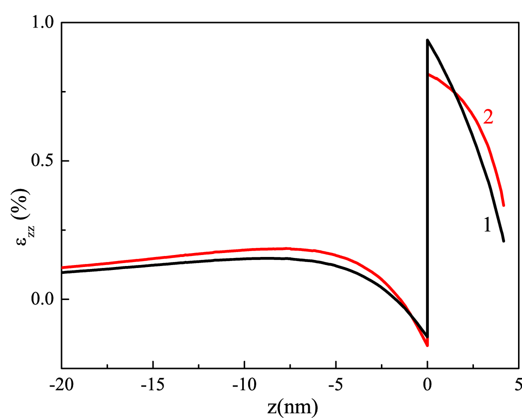

Fig. 6. The same as in Fig. 5, but for the strain tensor component ε_{zz}

component ε_{zz} has the opposite sign (Fig. 4): the substrate near the heterojunction undergoes compressive strains in the heterostructure growth direction, whereas nanoislands undergo the action of stretching strains. Moreover, the ε_{zz} component changes its sign in the substrate depth. At a distance of the order of the island height, the stretching strains have the maximum value, $\varepsilon_{zz} \approx 0.17\%$; then, they gradually decrease toward the substrate depth.

Qualitatively, the distributions of ε_{xx} (ε_{yy}) and ε_{zz} in heterostructures with islands characterized by a uniforn component content have the same features as in the case considered above. To elucidate the quantitative effect of non-uniformity in the distribution of elastic stress fields over heterostructures, let us consider the profiles of the tensor components ε_{ii} along the Oz-axis (Figs. 5 and 6).

As is seen from Fig. 5, the compressive strains ε_{xx} in the lower part ($z < h/2$) of non-uniform quantum dots are smaller by absolute value than the corresponding values in uniform islands. The maximum difference is observed near the pyramid base, being equal to $\Delta\varepsilon_{xx} \approx 0.45\%$. Approximately at the middle of the quantum dot height, the component ε_{xx} is identical in the islands of both types and equals $\varepsilon_{xx} \approx 1.4\%$. In the upper part of a quantum dot ($z > h/2$), the nanoislands with a non-uniform germanium distribution turn out more deformed, with the difference reaching its maximum near the pyramid vertex, where $\Delta\varepsilon_{xx} \approx 0.25\%$.

Islands with a non-uniform component content induce larger stretching strains ε_{xx} in the silicon substrate than uniform islands do. The maximum difference is reached near the heterojunction and amounts to $\Delta\varepsilon_{xx} \approx 0.2\%$. At the substrate depth $z \sim h$, this difference is practically equal to zero.

The effect of non-uniformity also manifests itself in a similar way in the profiles of the strain tensor component ε_{zz} (Fig. 6). In particular, in the lower third of the quantum dot height ($z < h/3$), stretching strains in uniform islands turn out larger than the corresponding values in non-uniform quantum dots, with the maximum difference attaining $\Delta\varepsilon_{zz} \approx 0.13\%$ near the base. In the upper section of nanoislands, the inverse relation takes place; namely, non-uniform islands undergo larger stretching strains, and the maximum difference equals $\Delta\varepsilon_{zz} \approx 0.14\%$ near the vertex. In contrast to the case of the tensor components ε_{xx} and ε_{yy}, the difference between the components ε_{zz}

for the considered types of quantum dots survives at distances $z \sim 4h$ in the substrate depth.

The obtained spatial dependences $\varepsilon_{ii}(x, y, z)$ $(i = x, y, z)$ were used to evaluate the average strain values over the quantum dot volume $V_{\rm QD}$,

$$\langle \varepsilon_{ii} \rangle = \int\limits_{V_{\rm QD}} \varepsilon_{ii}(x, y, z) dV. \tag{14}$$

The results of calculations showed that the nanoislands with a uniform component content turn out more strained than the non-uniform ones. The average strain values in them are $\langle \varepsilon_{zz} \rangle \approx 0.66\%$, and $\langle \varepsilon_{xx} \rangle \approx -1.4\%$ in uniform islands against $\langle \varepsilon_{zz} \rangle \approx 0.63\%$ and $\langle \varepsilon_{xx} \rangle \approx -1.1\%$ in non-uniform ones. The origin of such differences consists in weaker local strains in non-uniform quantum dots in the region near their bases, which provides the main contribution at the averaging.

As was indicated above, strains can cause changes of the energy bands in heterostructures. The results obtained in this work testify that the main differences between the elastically deformed states of uniform and non-uniform nanoislands are observed in their bulk. Therefore, the largest variations of the energy structure are to be expected in quantum dots. In heterojunctions of the second type, to which the junction Si–Ge belongs (see the inset in Fig. 7), it is holes that are localized in the quantum dots. Therefore, the non-uniformity in this region has to reveal a dominating influence on the valence band bottom. To confirm this conclusion, the energy bands in the examined heterostructure were calculated in the deformation potential approximation. The change in the valence band bottom induced by strains was calculated according to the relation

$$\delta E_V = aS_h - \frac{bS_b}{2} + \frac{\Delta_0}{3}, \tag{15}$$

where a and b are the constants of the deformation potential for the valence band, Δ_0 is the spin-orbit splitting, and S_h and S_b are the hydrostatic and biaxial strains, respectively, which are defined as follows:

$$S_h = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}, \tag{16}$$

$$S_b = 2\varepsilon_{zz} - \varepsilon_{xx} - \varepsilon_{yy}. \tag{17}$$

The results obtained testify (Fig. 7) that, in nanoislands with a uniform germanium content distribution,

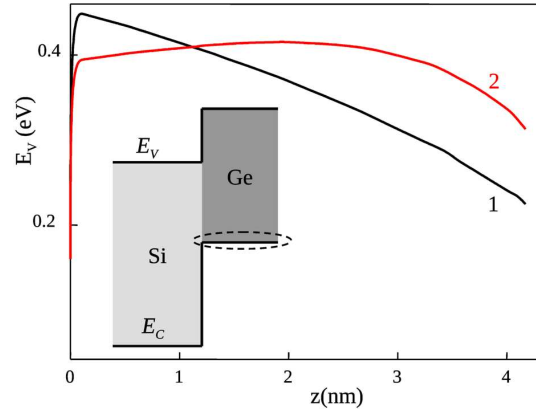

Fig. 7. Profiles $E_V(z)$ of the valence band bottom energy in nanoislands with uniform (*1*) and non-uniform (*2*) component contents. The inset illustrates the band diagram of the $Si_{1-x}Ge_x$ heterojunction; the region depicted in the main figure is outlined by a dashed curve

misfit strains give rise to an increase of the valence band bottom near the heterojunction Si–$Si_{1-x}Ge_x$ (curve *1*). Therefore, the maximum of hole density is observed in those quantum dots near the pyramidal island base. In non-uniform nanoislands, the maximum of E_V is attained approximately at the middle of their height (curve *2*). Hence, in quantum dots with a non-uniform content distribution, one should expect that a redistribution of the hole concentration would take place with a shift of its maximum toward the pyramid vertex. Moreover, the changes in the dependence $E_V(x, y, z)$ induced by the content non-uniformity would also stimulate modifications in the energy spectrum of charge carriers, which will make a contribution to the formation of the properties of heterostructures.

4. Conclusions

To summarize, the elastic strain fields in SiGe heterostructures with quantum dots synthesized following the Stranski–Krastanov growth mode were calculated. The results of calculations revealed a difference between the elastically deformed states of nanoislands with uniform and non-uniform distributions of silicon and germanium contents over their volume. The calculations testify that the non-uniformity of the contents of components changes the spatial distributions of strain tensor components and diminishes their magnitudes in quantum dots. Using the modifi-

cation of the valence band bottom energy as an example, the influence of the redistribution of germanium in nanoislands on the properties of SiGe heterostructures is demonstrated.

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ПРУЖНІ ДЕФОРМАЦІЇ
В SiGe-ГЕТЕРОСТРУКТУРАХ З КВАНТОВИМИ
ТОЧКАМИ НЕОДНОРІДНОГО СКЛАДУ

Р е з ю м е

Методом скінченних елементів розраховано розподіли пружних деформацій в гетероструктурах SiGe з квантовими точками. Досліджено вплив неоднорідного розподілу германію всередині наноострівців на просторові залежності та величину пружних полів. Показано, що квантові точки сталого складу характеризуються більшими напруженнями порівняно з неоднорідними наноострівцями.