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Elastic interaction of quantum disks in hybrid QD/NW structures

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The elastic interaction of quantum disks (QDs) in a nanowire (NW), i. e., in a hybrid QD/NW structure with sharp heterointerfaces, is considered for the first time. Within the framework of the defect micromechanics approach, the energy of QD pair interaction is established and it is demonstrated that for QDs with a lattice misfit of the same sign, a zone of attraction to each other appears, depending on the ratio of the QD axial size to the NW radius. The discovered effect should be taken into account when choosing the modes of formation of hybrid QD/NW structures and in models explaining their properties.

Keywords: nanowire (NW), quantum disk (QD), QD/NW hybrid structure, lattice mismatch, dilatation inclusion, strain energy.

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Currently, hybrid semiconductor structures comprising both nanowires (NWs) and quantum dots (QDTs) or quantum disks (QDs) attract attention of a wide circle of researchers (see, e. g., reviews [1,2]). This is caused by that such objects possess high structural perfectness which allows the quantum effects inherent to QDTs, QDs and NWs to be fully realized free of undesired additional influence of crystal lattice defects arising in planar semiconductor heterostructures.

QDTs and QDs may be incorporated into NW hybrid structures in different ways [3]: they may be located on the NW surface [4], fully embedded in the NW material [5–7] or occupy the entire NW cross section [8–10]. In the last case just analyzed in this work, axial QD/NW structures very promising for practical use in electronics [1] and photonics [2] are considered.

QDTs and QDs are NW regions with modified chemical compositions and structures and, hence, with physical properties different from those of the remaining part of the material. For further analysis, it is important whether there is a lattice misfit

$$\varepsilon_m = \frac{a_{\mathrm{QD}} - a_{\mathrm{NW}}}{a_{\mathrm{NW}}}, \tag{1}$$

where a_{QD} and a_{NW} are the crystal lattice parameters in the QD (or QDT) bulk and NW bulk, respectively. For simplicity, let us restrict ourselves to the dilatation (equi-axis) misfit characteristic of cubic-cell materials, for instance, A_3B_5 semiconductors with the sphalerite structure or Si and Ge with the diamond structure.

It is well known that lattice misfit arising in epitaxial growth of heterostructures is caused by formation in the material of elastic strains and mechanical stresses that, in their turn, modify the semiconductor properties and also give rise to dislocation defects in the course of stress relaxation [11]. Formation of dislocations in hybrid QD/NW heterostructures is hindered due to geometric restrictions, however, strain energy induced by the lattice misfit should be taken into account in considering such objects. This is just why this paper is devoted to the analysis of the pair elastic interaction of QDs in NW.

In the scope of the continuum mechanics approach, misfit ε_m gets the meaning of *eigenstrain* [12], and QD appears to be a finite-length elastic cylindrical inclusion. Earlier a number of problems were considered for determining characteristics (stresses and energies) of such inclusions in an infinite cylinder serving as an adequate model of NW. A review of the obtained results with references to primary sources is given in our recent paper [13] where it is noticed that inclusions with sharp and gradual variations in the eigenstrain along the cylinder axis were considered for the cases of the material elastic isotropy and transversal isotropy. In addition, elastic characteristics of single interfaces (transient regions) subdividing the cylinder into parts with constant eigenstrains [13–15] were studied. The control of the chemical composition and stressed state of such transient regions is important for NWs with axial heterostructures [14,16].

Fig. 1 presents a schematic picture of two interacting dilatation inclusions DI1 and DI2 in an elastically isotropic cylinder with radius a. The inclusion sizes (QD thicknesses) in the axial direction are h_1 and h_2, while the distance between them is L. Eigenstrain components ε^*_{ij} for each inclusion are defined by misfit $\varepsilon_m^{(1)}$ or $\varepsilon_m^{(2)}$. For instance, the relevant formula for DI1 is

$$\begin{aligned}\varepsilon^{*(1)}_{rr}(z) &= \varepsilon^{*(1)}_{\varphi\varphi}(z) = \varepsilon^{*(1)}_{zz}(z)\\ &= \varepsilon_m^{(1)} H\big[\tilde{h}_1/2 - |\tilde{z}|\big] H[1-\tilde{r}],\end{aligned} \tag{2}$$

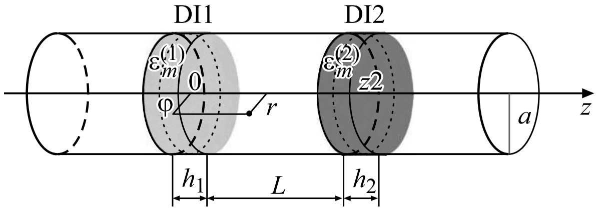

Figure 1. Schematic picture of interacting quantum disks (dilatation inclusions DI1 and DI2) in a nanowire represented as an elastically isotropic cylinder. The following inclusion parameters are shown: lattice misfits $\varepsilon_m^{(1)}$ and $\varepsilon_m^{(2)}$, axial dimensions h_1 and h_2, and coordinates $z_1 = 0$ and z_2 in the cylindrical frame of reference (r, φ, z).

where the cylindrical frame of reference (r, φ, z) is used; $\tilde{r} = r/a$, $\tilde{z} = z/a$, $\tilde{h}_{1,2} = h_{1,2}/a$, $H[p]$ is the Heaviside stepwise function.

In the scope of the elasticity theory, the boundary-value problem for an isolated dilatation inclusion in an elastically isotropic cylinder was considered in papers [13,15]. For instance, the following relation was obtained for stress tensor trace $\sigma_{ii}^{(1)}$ [13]:

$$\sigma_{ii}^{(1)} = -\frac{4G(1+\nu)\varepsilon_m^{(1)}}{1-\nu} H[\tilde{h}_1/2 - |\tilde{z}|] H[1-\tilde{r}] + \frac{8G(1+\nu)^2\varepsilon_m^{(1)}}{\pi(1-\nu)} \int\limits_0^\infty \frac{I_1(\beta) I_0(\tilde{r}\beta)}{\beta^2 I_0^2(\beta) - (\beta^2 - 2\nu + 2) I_1^2(\beta)} \times \sin\frac{\tilde{h}_1\beta}{2} \cos\beta\tilde{z}\, d\beta, \tag{3}$$

where G and ν are the shear modulus and Poisson coefficient of the cylinder material; $I_0(\xi)$ and $I_1(\xi)$ are the modified first-kind Bessel functions. The first right-hand term of relation (3) sets the tensor trace (triple hydrostatic component) of stresses in a dilatation inclusion located in infinite medium, which is zero outside the inclusion. The second right-hand term is generally nonzero and arises due to restrictions imposed on the stresses by the boundary conditions on the cylinder free surface. Just its contribution defines the interaction between the dilatation inclusions in the cylinder.

Generally, accumulated strain energy E induced by an arbitrary eigenstrain ε_{ij}^* may be found using the Mura relation [12]:

$$E = -\frac{1}{2} \int\limits_V \varepsilon_{ij}^* \sigma_{ij}\, dV, \tag{4}$$

where σ_{ij} are the stresses unambiguously defined by the eigenstrain and boundary conditions; the integration was performed over the entire volume of the elastic body under consideration.

In the task of determining the strain energy of a system of dilatation inclusions, relation (4) may be reduced to:

$$E = -\frac{\varepsilon_m^{(1)}}{2} \int\limits_{V^{(1)}} \sigma_{ii}^{(1)} dV - \frac{\varepsilon_m^{(2)}}{2} \int\limits_{V^{(2)}} \sigma_{ii}^{(2)} dV - \varepsilon_m^{(2)} \int\limits_{V^{(2)}} \sigma_{ii}^{(1)} dV, \tag{5}$$

where the first two right-hand terms are self energies $E^{(1)}$ and $E^{(2)}$ of isolated (but located inside the cylinder) dilatation inclusions DI1 and DI2, while the third term is the pair interaction energy $W(L)$ depending on distance L between the inclusions in the elastic cylinder; $V^{(1,2)} = \pi a^2 h_{1,2}$ are the inclusion volumes.

Calculations via relations (2), (3) and (5) give

$$E^{(1,2)} = \frac{2G(1+\nu)(\varepsilon_m^{(1,2)})^2}{1-\nu} V^{(1,2)} - \frac{16G(1+\nu)^2(\varepsilon_m^{(1,2)})^2 a^3}{1-\nu} \times \int\limits_0^\infty \frac{I_1^2(\beta)}{\beta^2 I_0^2(\beta) - (\beta^2 - 2\nu + 2) I_1^2(\beta)} \frac{1}{\beta^2} \left(\sin\frac{\tilde{h}_{1,2}\beta}{2}\right)^2 d\beta, \tag{6}$$

$$W(L) = -\frac{32G(1+\nu)^2 \varepsilon_m^{(1)} \varepsilon_m^{(2)} a^3}{1-\nu} \times \int\limits_0^\infty \frac{I_1^2(\beta)}{\beta^2 I_0^2(\beta) - (\beta^2 - 2\nu + 2) I_1^2(\beta)} \frac{1}{\beta^2} \sin\frac{\tilde{h}_1\beta}{2} \sin\frac{\tilde{h}_2\beta}{2} \times \cos\left(\tilde{L} + \frac{\tilde{h}_1}{2} + \frac{\tilde{h}_2}{2}\right)\beta\, d\beta, \tag{7}$$

where $\tilde{L} = L/a$. If $L = 0$, the inclusions adjoin each other. The case of overlapping inclusions was not considered.

The first right-hand term of relation (6) obtained for the first time in study [15] sets the volume–proportional energy of a dilatation inclusion in infinite medium, while the second term represents the reduction of the single inclusion energy because of screening the elastic fields by the cylinder free surface. By considering two dilatation inclusions in an infinite elastic medium, it is possible to make sure that their interaction energy is zero (if no overlapping of the inclusions takes place) since the hydrostatic stress component is absent outside the inclusion. Inside the cylinder, as relation (3) shows, this component is present, which gives rise to nonzero interaction of dilation inclusions expressed as (7) and, hence, to elastic interaction of QDs in NW.

Fig. 2 presents the dependence of interaction energy W on distance L between the equal-sized dilatation QDs ($h_1 = h_2 = h$, $\varepsilon_m^{(1)} = \varepsilon_m^{(2)} = \varepsilon_m$) in the cylinder. One can see that QDs with arbitrary axial dimensions (the results were validated for $h \geqslant 0.05a$ that is 2.5 nm at $a = 50$ nm) exhibit a negative interaction energy at low L, then energy leaves the negative range with increasing L, and the energy maximum $W_{\max}(h)$ is observed in the range from $L \sim 0.65a$–$0.66a$ at $h \geqslant 2a$ to $L \sim 1.3a$ at $h \approx 0.1a$. The energy of interaction between two QDs becomes insensitive to parameter h at $h \geqslant 2a$. Moreover, it gets almost zero when QDs become spaced by $L \approx 2.5a$.

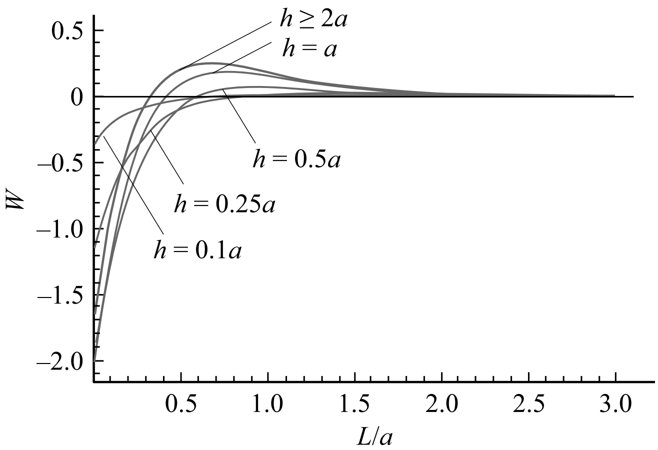

Figure 2. Energy of interaction between two identical quantum disks (dilatation inclusions) versus the distance between them along the nanowire (elastic cylinder) axis. The energy is given in the $G\varepsilon_m^2 a^3$ units where G is the shear modulus, ε_m is the QD/NW lattice misfit, a is the cylinder radius. The calculations were performed for the Poisson coefficient $\nu = 0.3$.

The obtained results open the way for further investigation of different relaxation processes in NWs leading to reduction of the NW strain energy, for instance, due to either redistribution and segregation of impurities or formation of misfit dislocations which is in the focus of our current interest. The effect of mutual attraction of QDs with three-dimensional dilatation eigenstrain revealed in this study raises the question on the dimensional stability of such heterostructures. Notice that the effect of attraction (repulsion) of point defects with dilatation eigenstrains of the same (or opposite) sign takes place in the case of their elastic interaction near the flat free surface [17] and also for dilatation defects located in an elastically anisotropic material [18].

Thus, a problem was set and solved on elastic interaction of quantum disks in hybrid QD/NW structures where the disk material possesses lattice misfit with the nanowire material. The quantum disks were represented as inclusions with dilatation eigenstrain incorporated in the nanowire material in the form of inserts. Earlier unknown effect of mutual attraction of quantum disks with dilatations of the same sign was revealed, and its intensity was shown to be defined by the reduced (relative to the NW radius) thickness of the interacting quantum disks.

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Conflict of interests

The authors declare that they have no conflict of interests.

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