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General approach to the calculation of elastic properties of axially symmetric quantum dots in nanowires

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A general approach to the calculation of elastic fields and energies of quantum dots (QDs) featuring dilatational eigenstrain and positioned along the symmetry axis of a nanowire (NW) is examined. The problem of elastic fields of an infinitely thin dilatational disk buried completely in a matrix in the form of a NW, which is represented by a straight infinitely long elastic cylinder with a constant radius, is solved for this purpose within the classical linear elasticity theory. It is demonstrated how an analytical solution for a dilatational disk may be used to calculate the elastic properties of axially symmetric QDs of various shapes in hybrid QD/NW nanostructures.

Keywords: dilatational disk, nanowire, elastic fields, accumulated strain energy, boundary-value problem of elasticity theory.

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Nanowires (NWs) are currently attracting increased research attention. Owing to their unique physical and chemical properties [1], NWs find application in numerous modern instruments and devices with fundamentally new functional capabilities [2,3].

Semiconductor NWs may also be used in practice to fabricate hybrid nanostructures incorporating quantum disks (nanodisks, NDs) or quantum dots (QDs) [4,5]. While NDs fill the entire NW cross section, QDs are buried completely in NWs (i.e., are surrounded by the NW material from all sides).

The elastic behavior of quantum disks in hybrid ND/NW structures, which is governed by the effect of misfit between the lattice parameters of ND and NW materials, has already been examined in [6,7]. It was demonstrated, e.g., that the screening influence of the free NW surface causes NDs with like-sign dilatation to attract each other at distances shorter than the NW radius [6].

A limited number of solutions in the special case with cylindrical QDs featuring uniaxial eigenstrain are available for QDs buried completely in NWs (see a brief review in [7]). Similar problems for QDs of other shapes have not been considered yet, although elastic characteristics of such objects in NWs are needed both for analysis of the structural evolution of hybrid QD/NW nanostructures and for examination of their physical and chemical properties. This is largely attributable to the lack of analytical solutions for elastic fields and energies of these QDs in NWs.

An approach providing in opportunity to determine elastic fields and energies of axially symmetric QDs of a complex shape in NWs is detailed in the present study. This approach involves solving a boundary-value problem of the classical linear elasticity theory for a dilatational disk (DD) of a finite radius that is completely buried in a coaxial elastically isotropic straight infinitely long cylinder with a constant radius, which serves as a continuum mechanical model of an NW.

Figure 1 presents a schematic diagram of dilatational QDs of different possible shapes (spherical (a), cylindrical (b), and conical (c ones) positioned on the axis of symmetry of a cylindrical NW. Within material micromechanics, a dilatational QD is a region within an NW where a dilatational eigenstrain is specified [8]:

$$\varepsilon^*_{ii} = \varepsilon^* \delta(\Omega)$$
$$(i = x, y, z \text{ or } i = r, \varphi, z; \quad \text{no summation over } i), \tag{1}$$

where ε^* is the lattice misfit, $\delta(\Omega) = 1$ within a QD, and $\delta(\Omega) = 0$ outside of it.

The idea of the proposed approach consists in presenting the mentioned axially symmetric QDs as sets of infinitely thin DDs (see the examples of such „sample" disks for each QD shape in Fig. 1). The elastic QD parameters may then be presented in an integral form. For example, stress field σ_{ij} is

$$\sigma_{ij} = \int\limits_{z_1}^{z_2} {}^{d}\sigma_{ij}\big(r, z - z_0; c(z_0)\big)\rho(z_0)dz_0, \tag{2}$$

where integration is performed over the QD height (see the example in Fig. 1, c for a conical QD),

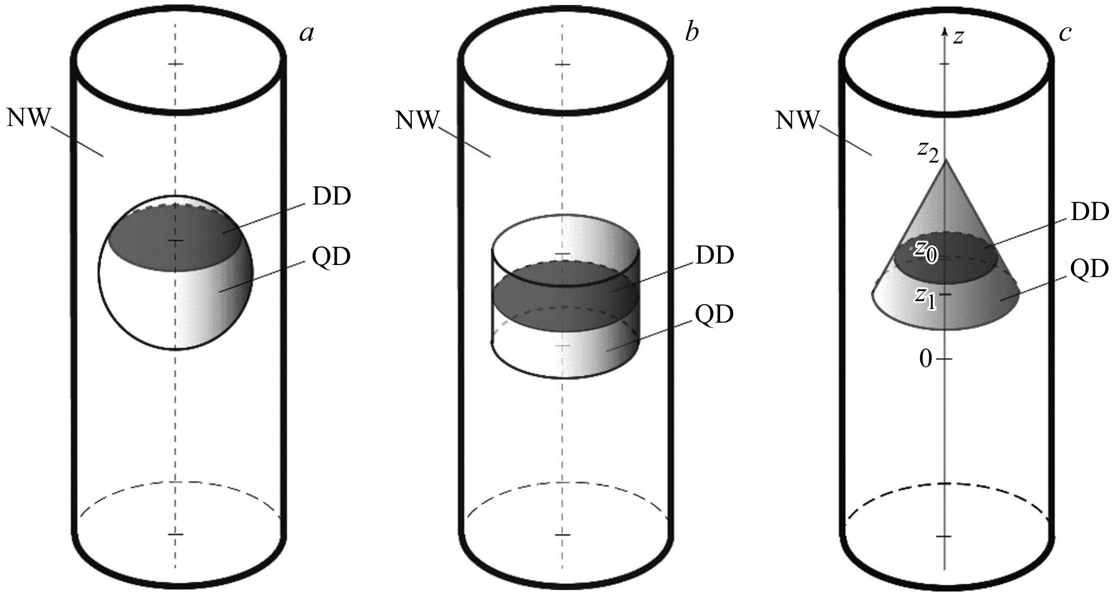

Figure 1. Axially symmetric QDs of various shapes in NWs: *a* — spherical, *b* — cylindrical, and *c* — conical QDs. A sample infinitely thin dilatational disk (DD) is shown. The integration limits and the position of the sample DD on (axial) coordinate axis z are also indicated for a conical QD.

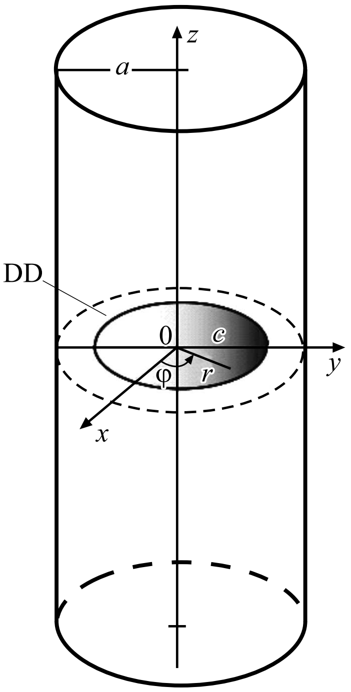

Figure 2. Dilatational disk (DD) with radius c in a cylinder with radius a. Cartesian (x, y, z) and cylindrical (r, φ, z) coordinate systems are shown.

${}^d\sigma_{ij}(r, z - z_0; c(z_0))$ is the stress field of a sample DD with radius $c(z_0)$ located at distance z_0 from the origin of coordinates, and $\rho(z_0)$ is the density of DD distribution along the NW axis (in the present study, its is assumed to be constant).

The DD eigenstrain may be written as [8]

$$ {}^d\varepsilon^*_{ii} = bH\left(1 - \frac{r}{c}\right)\delta(z), \tag{3}$$

where b is a dimensional coefficient accounting for the eigenstrain concentrated in the DD, $H(\dots)$ is the Heaviside step function, and $\delta(z)$ is the Dirac delta function. A relation similar to formula (3) may be used to determine the eigenstrain of axially symmetric QDs under the assumption of constant DD density $\rho = \varepsilon^*/b$:

$$\varepsilon^*_{ii} = \int_{z_1}^{z_2} {}^d\varepsilon^*_{ii}(r, z - z_0; c(z_0))\rho dz_0$$

$$= \int_{z_1}^{z_2} bH\left(1 - \frac{r}{c(z_0)}\right)\delta(z - z_0)\rho dz = \varepsilon^*\delta(\Omega). \tag{4}$$

In order to implement the proposed approach, one needs to determine the elastic characteristics of a sample DD in the geometry illustrated in Fig. 2 by solving a boundary-value problem of elasticity theory wherein boundary conditions on the stress-free lateral surface of an infinite cylinder are imposed on the elastic field of a source (i.e., DD).

If a DD is positioned in an infinite elastically isotropic continuum, its elastic fields are defined unambiguously by eigenstrain (3). The DD stresses in this case [10] were determined with the use of defect micromechanics relations [9]:

$$ {}^{\infty d}\sigma_{rr} = \frac{G(1+\nu)b}{1-\nu}\left[\frac{1}{c}J(1,0;1) - \frac{1}{r}J(1,1;0)\right] - \frac{2G(1+\nu)b}{1-\nu}H\left(1-\frac{r}{c}\right)\delta(z), \quad (5a) $$

$$ {}^{\infty d}\sigma_{\varphi\varphi} = \frac{G(1+\nu)b}{1-\nu}\frac{1}{r}J(1,1;0) - \frac{2G(1+\nu)b}{1-\nu}H\left(1-\frac{r}{c}\right)\delta(z), \quad (5b) $$

$$ {}^{\infty d}\sigma_{zz} = -\frac{G(1+\nu)b}{1-\nu}\frac{1}{c}J(1,0;1), \quad (5c) $$

$$ {}^{\infty d}\sigma_{rz} = -\frac{G(1+\nu)b}{1-\nu}\frac{\mathrm{sgn}(z)}{c}J(1,1;1), \quad (5d) $$

$$ {}^{\infty d}\sigma_{r\varphi} = {}^{\infty d}\sigma_{\varphi z} = 0. \quad (5e,f) $$

Here, G is the shear modulus, ν is the Poisson's ratio, $\mathrm{sgn}(z)$ is the sign function, and

$$ J(m,n;p) = \int_0^\infty J_m(\kappa)J_n(\kappa r/c)\exp(-\kappa|z|/c)\kappa^p d\kappa $$

are Lipschitz–Hankel integrals that are defined using Bessel functions of the first kind J_m and J_n [11].

The DD stress field in a cylinder (${}^d\sigma_{ij}$) may be plotted as a sum of DD stress field in an infinite medium ${}^{\infty d}\sigma_{ij}$ (5) and additional „image" stress field ${}^i\sigma_{ij}$:

$$ {}^d\sigma_{ij} = {}^{\infty d}\sigma_{ij} + {}^i\sigma_{ij}, \qquad i = x, y, z \text{ or } i = r, \varphi, z. \quad (6) $$

Additional field ${}^i\sigma_{ij}$ should be determined in a form having no singularity within a cylinder and ensuring that the following boundary conditions are satisfied on its lateral surface $r = a$:

$$ \left({}^{\infty d}\sigma_{rr} + {}^i\sigma_{rr}\right)\big|_{r=a} = 0, \quad (7a) $$

$$ \left({}^{\infty d}\sigma_{rz} + {}^i\sigma_{rz}\right)\big|_{r=a} = 0. \quad (7b) $$

The expression for image stress field ${}^i\sigma_{ij}$ is retrieved using the general solution obtained by Lur'e [12] for an elastic problem of an axisymmetrically loaded cylinder. Omitting the details of analytical calculation, we give the end result:

$$ {}^i\sigma_{rr} = \frac{2G(1+\nu)b}{(1-\nu)\pi a}\int_0^\infty \left[\beta\left(\tilde{C}_1(3-2\nu) - \tilde{D}_1\beta\right)I_0 + \frac{1}{\tilde{r}}\left(\tilde{C}_1(4\nu - \tilde{r}^2\beta^2 - 4) + \tilde{D}_1\beta\right)I_1\right]\cos\beta\tilde{z}\,d\beta, \quad (8a) $$

$$ {}^i\sigma_{\varphi\varphi} = \frac{2G(1+\nu)b}{(1-\nu)\pi a}\int_0^\infty \left[\tilde{C}_1\beta(2\nu-1)I_0 - \frac{1}{\tilde{r}} \times \left(4\tilde{C}_1(\nu-1) + \tilde{D}_1\beta\right)I_1\right]\cos\beta\tilde{z}\,d\beta, \quad (8b) $$

$$ {}^i\sigma_{zz} = \frac{2G(1+\nu)b}{(1-\nu)\pi a} \times \int_0^\infty \beta\left[\left(2\tilde{C}_1\nu + \tilde{D}_1\beta\right)I_0 + \tilde{r}\tilde{C}_1\beta I_1\right]\cos\beta\tilde{z}\,d\beta, \quad (8c) $$

$$ {}^i\sigma_{rz} = \frac{2G(1+\nu)b}{(1-\nu)\pi a} \times \int_0^\infty \beta\left[\tilde{r}\tilde{C}_1\beta I_0 + \left(2\tilde{C}_1(\nu-1) + \tilde{D}_1\beta\right)I_1\right]\sin\beta\tilde{z}\,d\beta, \quad (8d) $$

$$ {}^i\sigma_{r\varphi} = {}^i\sigma_{z\varphi} = 0, \quad (8e,f) $$

where

$$ \tilde{C}_1 = I_1^*\tilde{t}/\left[\beta^2 I_0^2 - (\beta^2 - 2\nu + 2)I_1^2\right], $$

$$ \tilde{D}_1 = -\tilde{C}_1\left[\beta^2 I_0 K_0 + \left(\beta^2 - 2\nu + 2\right)I_1 K_1 + 2\nu - 2\right]/\beta, $$

$I_1^* = I_1(\tilde{t}\beta)$, $I_0 = I_0(\tilde{r}\beta)$ and $I_1 = I_1(\tilde{r}\beta)$ are modified Bessel functions of the first kind, $K_0 = K_0(\beta)$ and $K_1 = K_1(\beta)$ are modified Bessel functions of the second kind (Macdonald functions), $\tilde{t} = c/a$, $\tilde{r} = r/a$, $\tilde{z} = z/a$, $\beta \geqslant 0$, and a is the cylinder radius that was introduced above.

Summing up the determined image stress field and the DD stress field in an infinite medium in accordance with formula (6), we obtain the sought-for result for DD stresses in an elastically isotropic cylinder. Figure 3, *a* illustrates the application of the obtained analytical solution in plotting a map of radial DD stress ${}^d\sigma_{rr}$ for which boundary condition (7a) is satisfied. The map of radial DD stress ${}^{\infty d}\sigma_{rr}$ for an infinite medium is shown in Fig. 3, *b* for comparison. Similar maps (not shown here) were plotted for the other stress tensor components specified by formulae (5) and (8).

The obtained solution allows one to calculate the accumulated elastic strain energy for a DD. This energy is calculated using the Mura formula [9]:

$$ {}^dE = -\frac{1}{2}\int_V \sigma_{ij}\varepsilon_{ij}^* dV = -\frac{1}{2}\int_V \left({}^{\infty d}\sigma + {}^i\sigma\right)bH \times \left(1-\frac{r}{c}\right)\delta(z)dV = {}^{\infty d}E + {}^{id}E, \quad (9) $$

where ${}^{\infty d}E$ is the DD energy in an infinite medium, ${}^{id}E$ is a correction due to the screening influence of the free cylinder (NW) surface, and integration is performed over the entire cylinder volume (V).

In virtue of the singular DD model, term ${}^{\infty d}E$ is formally infinite, which is unphysical. Instead, we consider a sufficiently thin DD with a finite thickness $h \ll c$. The following formula for the energy of a cylindrical dilatational inclusion with a limited height may be used in this case [13]:

$$ {}^{\infty d}E \approx \frac{2G(1+\nu)\varepsilon^{*2}}{1-\nu}\pi c^2 h. \quad (10) $$

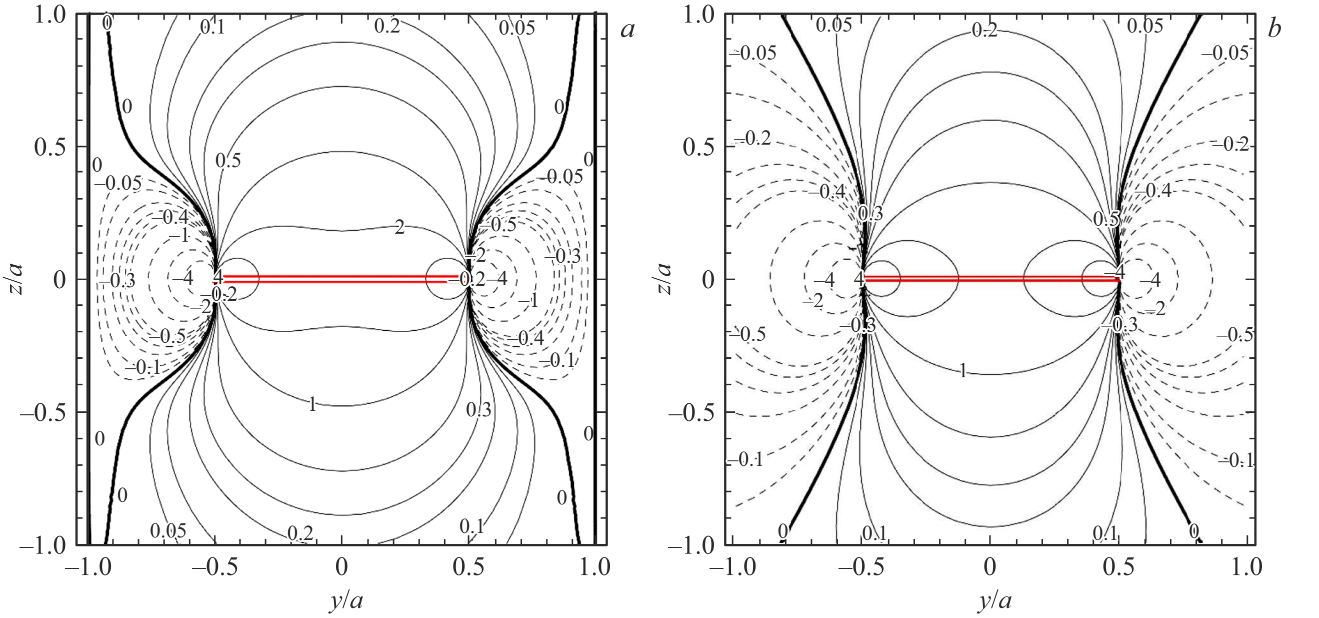

Figure 3. Maps of radial stresses of a dilatational disk in plane $y{-}z$. a — ${}^{d}\sigma_{rr}$ in a cylinder, b — ${}^{\infty d}\sigma_{rr}$ in an infinite medium. The double red line denotes the cross section of the dilatational disk (a color version of the figure is provided in the online version of the paper). Stresses are given in units of Gb/a; $\nu = 0.3$.

Term ${}^{id}E$ may be calculated without introducing the assumption of finiteness of the DD thickness. The result is

$$ {}^{id}E = -\frac{4G(1+\nu)^2 b^2 c^2}{(1-\nu)a} \int\limits_0^\infty \frac{I_1^{*2}}{\beta^2 I_0^2 - (\beta^2 - 2\nu + 2)I_1^2} d\beta. \tag{11} $$

One needs to take the relations between parameters ε^*, h, and b into account to perform qualitative and quantitative analysis of energy ${}^{d}E$ of a DD in an NW. It is fair to assume that an atomically thin DD (atomic cluster) has $h = l$, where l is the lattice parameter under condition $l \ll a$. Assuming that b specifies the variation of the lattice parameter in the DD plane, we find $\varepsilon^* = b/l$, which then yields the following expression for the energy of a thin DD in an NW:

$$ {}^{d}E \approx \frac{2G(1+\nu)\pi\varepsilon^{*2} a c^2}{1-\nu} \times \left(\tilde{\lambda} - \frac{2(1+\nu)\tilde{\lambda}^2}{\pi} \int\limits_0^\infty \frac{I_1^{*2}}{\beta^2 I_0^2 - (\beta^2 - 2\nu + 2)I_1^2)} d\beta \right), \tag{12} $$

where $\tilde{\lambda} = l/a$. It follows from our analysis that the effect of screening by the cylinder surface exerts only a weak influence on the total DD energy if $\tilde{\lambda}$ varies within reasonable limits (e.g., from 0.001 to 0.03). However, the influence of the free NW surface becomes decisive in the case of QDs of a finite height (Fig. 1) comparable to their radial dimension.

Thus, a general approach to the calculation of elastic fields of axially symmetric QDs in hybrid QD/NW nanostructures was developed. It was proposed that a QD should be treated as a dilatational inclusion for this purpose, while a NW should be regarded as an elastically isotropic straight infinite cylinder with a constant circular cross section. An Infinitesimally thin dilatational disk, which is buried completely in this cylinder and is coaxial with it, was introduced as a basic element that allows one to obtain solutions for QDs of various shapes. Analytical expressions for elastic fields and energies of this DD were found.

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Conflict of interest

The authors declare that they have no conflict of interest.

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