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Rapid Research Note

Interfacial Elasticity Corrections to Size-Dependent Strain-State of Embedded Quantum Dots

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Introduction Quantum Dots (QDs) have recently been the focus of several experimental and theoretical researchers due to the promise of improved and new opto-electronic properties [1]. Frequently, embedded QD structures (e.g. InAs/GaAs system), to preserve coherency, must accommodate large lattice mismatch. The ensuing elastic relaxation and the hydrostatic strain state within the QD structure are well known to impact its opto-electronic properties [2, 3]. Several works, of varying sophistication (both analytical and numerical), have focused on the "accurate" calculation of the strain state in buried quantum dots [4–8]. Recently, two papers have caught the present authors attention. Pan and Young [4] indicated significant difference in strain calculation when anisotropic elastic behavior is assumed compared to simplified isotropic elasticity. Further, a recent article by Ellaway and Faux [8] indicated (via atomistic simulations) that the elastic properties of QD are stain-dependent and such a consideration on strain calculation can result in a significant correction (of 16%) to the hydrostatic strain (in their article, for a buried spherical InAs/GaAs QD). In this communication, we show that the so-far unconsidered interfacial elastic properties can also significantly alter the strain calculations; the exact correction sensitively being dependent upon the size of the QD structure and the interfacial elastic constants. We find that the correction resulting from interfacial elasticity is comparable to that due to either anisotropic or strain-dependency effects.

Classical elasticity (on which most of the previous works are based) does not admit intrinsic size dependence in the elastic solutions of embedded inhomogeneities. For structures with sizes > 50 nm, typically, the surface-to-volume ratio is negligible and the deformation behavior is governed by classical bulk strain energy. Currently, no formulation exists which combines interface elasticity with bulk elasticity to analyze embedded inclusions. Eshelby's [9] celebrated formalism, often used in QD literature, is based entirely on classical bulk elasticity. In this communication (using a variational approach) we derive a general expression for the correction in hydrostatic strain due to interfacial elasticity (for an embedded spherical quantum dot). Despite the lack of precise data, we are able to show (using InAs/GaAs as an example system) that inclusion of interfacial elasticity effects can result in *minimum* corrections between 1.8% and 12% in the typical size range of QD structures (2–20 nm).

Formulation A generic and mathematical exposition on surface/interface elasticity has been presented by Gurtin and co-workers [10]. The interface/surface stress tensor, σ^{S}, is related to the deformation dependent surface energy, $\Gamma(\varepsilon_{\alpha\beta})$ by

$$\sigma^{\mathrm{S}}_{\alpha\beta} = \tau_0 \delta_{\alpha\beta} + \partial\Gamma/\partial\varepsilon_{\alpha\beta}\,. \tag{1}$$

Here, $\varepsilon_{\alpha\beta}$ is the 2×2 strain tensor for surfaces, $\delta_{\alpha\beta}$ represents the Kronecker delta for surfaces while τ_0 is the deformation independent surface/interfacial tension. The equilibrium and constitutive equations for isotropic case can be summarized as follows [10]:

– in the bulk: $\sigma^{\mathrm{B}}_{ij,j} = 0; \qquad \sigma^{\mathrm{B}}_{ij} = \lambda\delta_{ij}\varepsilon_{kk} + 2\mu\varepsilon_{ij},$ (2a, b)

– on the surface/interface:

$$\sigma^{\mathrm{B}}_{\beta\alpha} n_\beta + \sigma^{\mathrm{S}}_{\beta\alpha,\beta} = 0\,; \qquad \sigma^{\mathrm{B}}_{ji} n_j n_i = \sigma^{\mathrm{S}}_{\alpha\beta}\varkappa_{\alpha\beta},$$

$$\sigma^{\mathrm{S}}_{\beta\alpha} = \tau_0\delta_{\beta\alpha} + 2(\mu_{\mathrm{S}} - \tau_0)\,\varepsilon_{\beta\alpha} + (\lambda_{\mathrm{S}} + \tau_0)\,\varepsilon_{\gamma\gamma}\delta_{\beta\alpha}\,. \tag{2c–e}$$

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Here, $\varkappa$ and μ are the Lamé constants for the isotropic bulk material. Isotropic interfaces or surfaces can be characterized by surface Lame' constants λ_S, μ_S. Here, $\varkappa_{\alpha\beta}$ represents the curvature tensor of the surface/interface, n_α is the normal vector on the interface. Where applicable, superscripts B and S indicate bulk and surface, respectively. It is to be noted that only certain strain components appear within the constitutive law for surfaces due to the 2×2 nature of the surface stress tensor (i.e. strains normal to the surface are excluded). Thus, the Greek indices take on values 1 and 2 while Latin subscripts adopt values 1 through 3.

Consider now a spherical QD, of radius R_0, located in an infinite semiconductor matrix and undergoing a dilatation eigenstrain, i.e., $\varepsilon^*_{11} = \varepsilon^*_{22} = \varepsilon^*_{33} = \varepsilon^*$. The bulk and surface elastic energy densities of an inhomogeneity-matrix system can be given as

$$\Psi^{\mathrm{B}}_{\Lambda} = \tfrac{1}{2}\lambda_{\Lambda}(\varepsilon_{ii})^2 + \mu_{\Lambda}\varepsilon_{ij}\varepsilon_{ij} - 3K_{\Lambda}\varepsilon^*\varepsilon_{ii}; \quad \Psi^{\mathrm{S}} = \int_S \mathrm{d}S \int_0^{\varepsilon^{\mathrm{S}}_{ij}} \sigma^{\mathrm{S}}_{ij}\mathrm{d}\varepsilon^{\mathrm{S}}_{ij}\,, \tag{3}$$

where Λ represents either the inhomogeneity "I" or the matrix 'M', K_Λ is the bulk-modulus ($= \lambda_\Lambda + \mu_\Lambda/3$) for isotropic elastic solids, ε^* the eigenstrain which is finite in the inhomogeneity and zero outside of it. The free energy of the spherically symmetric system, in the presence of interface elasticity, can then be written as

$$\Pi = 4\pi \int_0^{R_0} r^2 \Psi^{\mathrm{B}}_{\mathrm{I}}\,\mathrm{d}r + 4\pi R_0^2 \int_0^{\varepsilon^{\mathrm{S}}_{ij}} \sigma^{\mathrm{S}}_{ij}\,\mathrm{d}\varepsilon^{\mathrm{S}}_{ij} + 4\pi \int_{R_0}^{R_\infty} r^2 \Psi^{\mathrm{B}}_{\mathrm{M}}\,\mathrm{d}r\,. \tag{4}$$

The Euler-Lagrange equations and the appropriate boundary conditions are obtained by setting the variation of the free energy to be zero, i.e. $\delta\Pi = 0$. The spherically symmetric problem leads to a displacement field that is radially symmetric, i.e., $u = u(r)$. Using the strain-displacement relation in spherical coordinate basis, Eq. (4), the constitutive Eqs. (2), and taking the variation of the total energy with respect to the displacement fields, we obtain Eq. (5a): Euler's equation for the integrand in both the inhomogeneity and matrix domains; Eq. (5b): the equilibrium of the bulk and surface forces at the interface, and finally Eq. (5c): the natural boundary condition:

$$r^2\partial^2 u/\partial r^2 - 2r\partial u/\partial r - 2u = 0\,, \tag{5a}$$

$$\sigma^+_{rr} - \sigma^-_{rr} = (2\sigma^{\mathrm{S}}_{\theta\theta}/R_0)_{r\to R_0}\,, \tag{5b}$$

$$\sigma_{rr}|_{r\to\infty} = 0\,. \tag{5c}$$

The general solutions to the differential equation of Eq. (5a) are simply r and $1/r^2$. The proper solutions of Eqs. (5a–5c) are obtained by satisfying the following additional constraints: (i) at the center of the QD, $u(r)$ must approach zero; (ii) at $r \to \infty$, $\varepsilon \to 0$, and finally (iii) displacements must be continuous across interface i.e. $u^+(r \to R_0) = u^-(r \to R_0)$. The final solution, after the necessary mathematical manipulation, is then

$$\varepsilon_{rr} = (3K_{\mathrm{I}}\varepsilon^* - 2\tau_0/R_0)/(4\mu_{\mathrm{M}} + 3K_{\mathrm{I}} + 2K_{\mathrm{S}}/R_0)\,, \tag{6}$$

where $K_{\mathrm{S}} = 2(\mu_{\mathrm{S}} + \lambda_{\mathrm{S}})$ is introduced in this article to be the "surface modulus". Note that the interfacial elasticity effects enter the equations via K_{S} and τ_0 weighted appropriately by the curvature ($1/R_0$) of the QD. Making R_0 arbitrarily large can trivially retrieve the classical solution. Another interesting feature of our solution is that the hydrostatic strain within the QD structure is now size dependent unlike the classical elasticity analysis of previous researchers (e.g. [4–8]).

Results and Discussion Our formulation is applied to InAs/GaAs system. The eigenstrain (or lattice mismatch strain) is 6.685% [8]. The bulk elastic constants used are $\{\mu_{\mathrm{InAs}} = 19, K_{\mathrm{InAs}} = 57.1\}$ GPa and $\{\mu_{\mathrm{GaAs}} = 32.9, K_{\mathrm{GaAs}} = 75.4\}$ GPa. For the interfacial properties one needs deformation dependent constants K_{S} and deformation independent interfacial tension, τ_0. While the latter is known experimentally [11], the former is not known precisely. Nevertheless, we can provide the *lower bound* on the corrections to the hydrostatic strain calculated by classical methods via a simple consideration. A glance at Eq. (6) indicates that ignoring the surface modulus K_{S}, will result in the underestimation of the strain. Thus, incorporating interfacial elasticity only through τ_0 (neglecting K_{S}) will result in a lower bound on the actual hydrostatic strain. We use $\tau_0 = 0.72$ J/m^2 (taken from Ref. [11]) in our calculations. In Fig. 1, the absolute value of the percentage correction

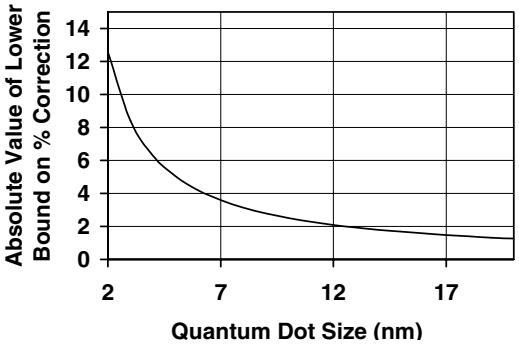

Fig. 1. Lower bound on strain correction

to the classical solution is plotted with respect to varying QD size. Clearly, the interfacial effects can add a substantial correction to the elastic state especially at smaller sizes. Interestingly the corrections we suggest due to interfacial effects are comparable to both anisotropic effects [4] and strain-dependent modulus effect [8].

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