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Elastic and piezoelectric field around a quantum dot with interface effect

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ABSTRACT

Piezoelectric field is closely related to the elastic field, so it is important for the calculation of piezoelectric field to include the size-dependent interface effect for the interface in nanostructures. This work adopts the semi-coupled model to find the elastic and piezoelectric field for weakly electromechanical coupled materials (GaAs) with the consideration of interface effect. Close-form solutions are derived and numerical results are also provided to show that the piezoelectric potential in the matrix depends on the interface elasticity, the radius and stiffness of the quantum dot. Especially, it is demonstrated that the piezoelectric potentials with different interface elasticity parameters are distinct compared with the classical solution near the interface. When the interface elasticity parameter is positive, the interface effect weakens the piezoelectric effect in the material by decreasing the value of the piezoelectric potential and vice versa. The piezoelectric potential concentration ratio calculated by this work with the consideration of interface elasticity is close to 10% different from the classical solution. Such amount of difference is appreciable in the design and fabrication of nanostructures and the effect due to interface elasticity should not be neglected.

1. Introduction

Many III-V semiconductor materials (e.g. GaAs, AlN and etc.) exhibit piezoelectric behaviors. By taking the advantage of the piezoelectric effect, these semiconductor materials are good candidates of sensors, actuators or for energy-harvesting applications [1–3]. Furthermore, in modern technology, they could be fabricated as semiconductor nanostructures, such as quantum dots (QDs), quantum wells (QWs) or quantum wires (QWRs). When a QD is buried in a surrounding matrix, an elastic field will be generated due to lattice mismatch or thermal expansion difference between the QD and surrounding matrix, which will induce an piezoelectric field in the structure. Therefore, theoretical studies on the elastic and piezoelectric field of nanostructures are helpful for the design and fabrication of nanostructures. Typically in the physics community for the prediction of the piezoelectric field, the elastic field is first solved and then it is used to obtain the polarization field which calculates the piezoelectric potential and electric field afterwards. Davies [4] formulated close-form solutions to the elastic and piezoelectric field in an infinite region of isotropic GaAs matrix due to a spherical InAs QD under hydrostatic misfit strain. Taking advantage of the celebrated work of Eshelby [5] and extended work of Downes et al. [6], Davies [4] also proposed solution strategies for the piezoelectric field in an isotropic matrix around any QD shapes. It should be noted that such semi-coupled or sequentially-coupled model between strain and piezoelectric field only works well where the electromechanical coupling in the semiconducting materials (e.g. GaAs) is weak. Pan [7] compared the different results of the piezoelectric field using semi-coupled and fully-coupled method. Furthermore, Pan [8] formulated the piezoelectric field in anisotropic GaAs matrix due to a QD under hydrostatic misfit strain. Recently, Chu et al. [9] proposed a general perturbation method for inhomogeneities in anisotropic and piezoelectric solid with applications to quantum-dot nanostructures. On the other hand, numerical solutions to the elastic and piezoelectric field have also been used compared to the analytical solutions. Jogai [10] numerically solved the three dimensional strain and piezoelectric field in InN/AlN wurzite QDs. Liu et al. [11] obtained the strain distribution in truncated GaN/AlN hexagonal QD by finite element analysis and then the piezoelectric field by numerical calculations afterwards.

Based on classical continuum mechanics, aforementioned works treated the interface between the QD and matrix traditionally where all physical quantities are continuous across the interface. In the design and fabrication of nanostructures, the critical length of the nanostructure drops down to several nanometers and classical continuum mechanics could not treat the subtle behavior of the interface (and surface) appropriately. In this case, surface/interface stress should be considered. Gurtin and Murdoch [12,13] first formulated the surface/interface stress as a strain-dependent term so the stress field is actually discontinuous across it. Miller and Shenoy [14] introduced the concept of surface stiffness and demonstrated the size-dependent elastic

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properties of nano-sized structure members. Moreover, intrinsic surface/interface properties could be obtained through molecular dynamics simulations [14–17]. Furthermore, it has been demonstrated that the elastic field in nanostructures differs from classical solutions due to the size-dependent surface/interface effect [18–21].

Since piezoelectric field is closely related to the elastic field, it is also important for the calculation of piezoelectric field to include the size-dependent interface effect for the interface between the QD and matrix in nanotechnology. For simplicity, isotropic material properties are assumed in this work as Refs. [4,7]. In fact, such simple assumption of isotropic material properties is used often for anisotropic semiconductors to obtain close-form solutions or just to simplify the derivation process in the literature. For instance, Sharma and Ganti [22] derived the analytical solution to the size-dependent elastic state of embedded InAs QD in GaAs matrix by assuming both the QD and matrix as isotropic materials. Shodja et al. [23] investigated the behavior of an edge dislocation in isotropic InAs core and GaAs matrix as a shell, while Ahmadzadeh-Bakhshayesh et al. [24] investigated the behavior of a screw dislocation in isotropic InAs core and InP matrix as a shell. However, the anisotropic material properties of semiconductors are still suggested to be used strictly for practical use. To focus on the importance of the size-dependent interface effect, this work adopts the semi-coupled model to find the elastic and piezoelectric field for weakly electromechanical coupled materials (such as GaAs). Compared with Refs. [4,7], our results indicate that interface elasticity can significantly alter the elastic and piezoelectric field at nano scales.

2. Methodology

2.1. Elastic field

In Fig. 1, a spherical InAs QD (Ω) with radius R_0 is buried in an infinite GaAs matrix (V). The interface between the QD and matrix is denoted by S. The QD is subjected to a dilatational eigenstrain ε^* due to lattice mismatch or thermal expansion difference between the QD and surrounding matrix.

From continuum mechanics, the stress field is governed by the stress equilibrium condition without body forces as:

$$\sigma_{ij,j} = 0. \tag{1}$$

The QD and matrix are both assumed to be isotropic materials. Therefore, the constitutive relationship between the stress and strain field are:

$$\sigma_{ij} = \lambda\varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij}, \tag{2}$$

where λ and μ are Lamé constants for isotropic materials; δ_{ij} is the Kroneker delta tensor. The Lamé constants of the QD and matrix are denoted as (λ_I, μ_I) and (λ_M, μ_M) respectively.

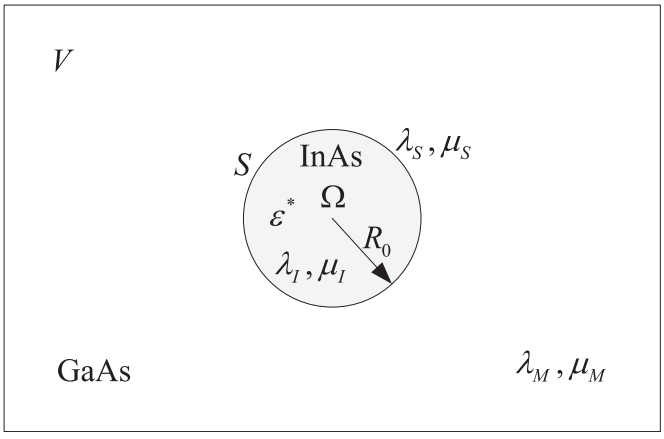

Fig. 1. Schematic view of a spherical InAs QD buried in an infinite GaAs matrix.

Since the size of QD is extremely small and its critical length drops down to several nanometers, the mechanical behavior of the interface between the QD and matrix should be considered to be size-dependent. Consider a linear constitutive relationship between interface stress and interface strain as [12,13]:

$$\sigma^s_{\alpha\beta} = \tau^0\delta_{\alpha\beta} + 2(\mu_S - \tau^0)\varepsilon^S_{\alpha\beta} + (\lambda_S + \tau^0)\varepsilon^S_{\gamma\gamma}\delta_{\alpha\beta}, \tag{3}$$

where λ_S and μ_S could be regarded as interface Lamé constants to describe the interface elasticity; τ^o is the residual interface stress under unstrained condition which is neglected in this work. It should be noted that the interface elastic property is extremely difficult to obtain by experiment so there is no such report on the values of λ_S and μ_S. However, molecular dynamics simulations indicate that λ_S and μ_S are between −10 N/m and 10 N/m for most metallic crystals and semiconductors [16,17,25]. Therefore, the interfacial elastic properties are simply assumed in this work.

Additionally, the interface between the QD and matrix is considered to deform coherently without slipping from the bulk material. In this case, the interface strain equals to the bulk strain so the displacement and strain field are continuous across the interface. However, the bulk stress field in the QD and matrix are discontinuous and the bulk stress state at the vicinity of the interface is determined from the interface stress [12,13]:

$$\sigma^s_{\alpha\beta,\beta} + [\![\sigma^b_{\alpha\beta}n_\beta]\!] = 0, \tag{4}$$

$$\sigma^s_{\alpha\beta}\kappa_{\alpha\beta} = [\![\sigma^b_{ij}n_in_j]\!], \tag{5}$$

where $\sigma^s_{\alpha\beta}$, $\sigma^b_{\alpha\beta}$ are the interface stress and bulk stress respectively; $\kappa_{\alpha\beta}$ is the curvature tensor and $[\![*]\!] = (*)_M - (*)_I$ denotes the quantity jump across the interface.

It should be noted that the interface stress tensor is a two-dimensional quantity and the strain normal to the interface is excluded. Thus, the Greek indices take the value of 1 or 2, while Latin subscripts adopt values from 1 to 3. Eq. (4) could be regarded as interface stress equilibrium equation similar to the bulk stress equilibrium equation of Eq. (1), while Eq. (5) could be regarded as the interface boundary condition.

In the current configuration, the displacement field is radically symmetric, so the only nonzero displacement component in spherical coordinate system is the radial displacement $u = u(r)$, and the strain field could be written as:

$$\varepsilon_{rr} = \frac{du}{dr};\ \varepsilon_{\theta\theta} = \varepsilon_{\phi\phi} = \frac{u}{r} \tag{6}$$

In case of the radically symmetric configuration, the strain and stress field should be also radically symmetric. Therefore, Eq. (5) of the interface boundary condition could be simplified as [18]:

$$[\![\sigma^b_{rr}]\!] = \frac{2\sigma^S_{\theta\theta}}{R_0}, \tag{7}$$

where σ^b_{rr} is given in Eq. (2) and $\sigma^S_{\theta\theta}$ is given in Eq. (3).

From Eqs. (1)–(6), the displacement field could be solved as:

$$u(r) = \begin{cases} \frac{K_I\varepsilon^*R_0 r}{2K_S + K_I R_0 + 4\mu_M R_0};\ r \le R_0 \\ \frac{K_I\varepsilon^*R_0^4}{(2K_S + K_I R_0 + 4\mu_M R_0)r^2};\ r \ge R_0 \end{cases} \tag{8}$$

where $K_I = 3\lambda_I + 2\mu_I$ and $K_S = 2\lambda_S + 2\mu_S$ are used to simplify the notation.

It can be seen from Eq. (8) that the displacement field inside the QD is proportional to the radius but it varies with an attenuating order of r^{-2} in the matrix.

The strain field is also obtained as: