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Exact piezoelectric solution for misfitted inclusion in finite spherical matrix: Applications to quantum dot core/shell crystals☆

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ABSTRACT

Piezoelectric behavior of quantum dot core/shell structures in zinc-blende and wurtzite crystals are investigated in the framework of linear piezoelectricity. Strains arising from lattice mismatch in the core/shell structure are modeled as eigenstrains resulting from size-mismatched inclusion embedded in a finite spherical piezoelectric medium. Assuming that the core/shell piezoelectric structure exhibits spherically-hexagonal anisotropy, an exact solution is obtained through the eigenvalue decomposition method and the analytical expressions of the electroelastic fields are found using appropriate boundary and continuity conditions. It is found that the electroelastic fields can become singular or vanish at the center of the core for certain cases of spherical anisotropy. The analytical solutions are verified with the finite element analysis (FEA) and found to be in excellent agreement. FEA for the case of rectilinear anisotropy was also performed which showed considerable difference from the spherically anisotropic analytical solution. The closed-form solution obtained in this work can be used for any two-layer piezoelectric structures having spherical geometry subjected to various electromechanical loads.

1. Introduction

Quantum dots (QDs) are nanocrystals that are widely used in electronic devices as semiconductors due to their distinct and unique characteristics (Hong et al., 2012). Among them, the nanoscale optoelectronic properties are utilized in fine tuning the electronic band structure to optimize the performance of optoelectronic devices. QD structures are often manufactured as core/shell assembly due to the chemical sensitivity of the core surface which leads to degradation of emission properties. Hence, the shell structures are fabricated to enhance the surface passivation (Lim et al., 2014). Since the core and the shell are often made from different materials with different lattice dimensions, the assembled QD core/shell structures can induce misfit strains. The misfit strains have a profound effect on the exciton dynamics and blinking properties which play an important role in determining the light emission performance. The induced strains can alter the theoretical prediction of the optoelectronic properties that are calculated from the first principle calculations. Hence, in order to better predict the optoelectronic properties, the elastic strains must be included in the Hamiltonian equations in calculating the electronic band structures which are usually calculated by the k · p method (Chuang and Chang, 1996; Park and Chuang, 1998). The purpose of this work is to provide a linear elasticity solution for a free-standing QD core/shell structure so that the misfit strains can be properly taken into account in quantum mechanical calculations (Park and Cho, 2011). The obtained solutions are applied to Cadmium Selenide/Cadmium Sulfide (CdSe/CdS) core/shell QD structures which come in the form of zinc-blende (ZB) or wurtzite (WZ) crystals. ZB crystals exhibit cubic material symmetry and show no piezoelectricity, whereas WZ crystals with hexagonal material symmetry show fully coupled piezoelectric effects. Therefore, a piezoelectric analysis is required in studying the electroelastic behavior of wurtzite crystal QDs since both the elastic and piezoelectric fields are equally important in understanding their optoelectronic properties. The physics community usually uses semicoupled models in analyzing piezoelectric fields in QDs wherein a purely elastic solution is first obtained through linear elasticity analysis which is then used to find the polarization field, and subsequently the electric potential and electric fields. Using this approach, the piezoelectric polarization induced by an elastic field was obtained for spherical, cuboidal, and pyramidal dots (Davies, 1998). However, Pan (2002) pointed out that the semicoupled model can give error especially for materials exhibiting strong piezoelectric coupling behavior. In this work, the electroelastic fields are obtained for QDs that are modeled as a misfitted inclusion in a finite spherical

☆ This paper is dedicated to the late Prof. S.-H. Yoo in his memory.

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matrix taking into account of fully-coupled piezoelectric effects (Pan, 2002).

In order to make these mathematical analyses simple as to yield a closed-form solution, we have assumed that the piezoelectric core and shell assembly exhibit spherically hexagonal anisotropy. This may not accurately model the actual QD crystals which show rectilinearly-cubic or rectilinearly-hexagonal anisotropy as in the bulk material. However, a simple closed-form solution may prove useful for researchers who are more familiar with quantum mechanical calculation rather than elaborate elasticity analysis. Thus, incorporating fully-coupled piezoelectricity, we have used the eigenvalue decomposition method and obtained a closed-form solution for the two-domain problem that can handle the misfit via displacement jump condition across the interface. Our solution matches exactly with that of a previous work whose solution was obtained using a different method for a single-domain piezoelectric sphere (Heyliger and Wu, 1998). Subsequently, our electroelastic solutions for various cases are verified with FEA simulations. To account for the misfit strain arising from lattice mismatch, Eshelby's eigenstrain concept was used with equivalent thermal strain in performing the FEA simulations.

Much theoretical works on eigenstrains induced by a lattice mismatch in QDs have been studied during the past two decades. Zero dimensional QDs are often embedded in a matrix or synthesized by coating the core structures with functional materials. Pyramidal and cubic structures embedded in an infinite matrix were examined analytically by using Green's function or Eshelby method (Downes et al., 1997). The analytical solutions introduced by Eshelby (1957) was extensively utilized in the framework of three dimensional elasticity. Subsequently, Green's function method was developed to obtain for arbitrary shapes. Using these methods, the strain distributions in the arbitrarily shape QDs were examined along various crystallographic directions, and the assumption of isotropy of QDs was demonstrated within a reasonable accuracy (Andreev et al., 1997). There also were endeavors incorporating atomistic effects to improve the theoretical predictions (Makeev and Madhukar, 2002). For sub 10 nm structures, the strain distribution including the surface effects are calculated which can reflect the size-dependent properties of QD structures (Sharma et al., 2003). The mechanical strain incorporating size-dependent effect was examined by comparing the calculations from non-local elasticity and classical elasticity. Extensive work in this area is well reviewed in an article by Maraganti and Sharma (2007). In comparison with a single quantum dot structure embedded in an infinite matrix, however, the theoretical work for a free-standing QD core/shell structure incorporating fully-coupled piezoelectric effect has not been as extensively addressed (Park and Cho, 2011).

The work herein provides the closed-form solution for the piezoelectric behavior arising in piezoelectric core/shell structure in the framework of classical linear elasticity. This work can contribute to the theoretical prediction of the optoelectronic properties and help in gaining deeper understanding of the optoelectronic behavior of QD devices. The solutions obtained can also be applied to any piezoelectric composite structures having spherical symmetry that arises in modeling practical devices such as sonar transducers.

2. Analytical solutions for misfitted piezoelectric inclusion in finite piezoelectric matrix

Considering the spherical symmetry of the problem at hands, the displacement, u_i, and the electric potential, Φ, depend only on the radial coordinate, R, such that

$$u_R = u_R(R), \quad u_\theta = u_\phi = 0$$
$$\Phi = \Phi(R). \tag{1}$$

In the absence of body force and body charge, the electroelastic governing equations can be written

$$\sigma_{ij,j} = 0,$$
$$D_{i,i} = 0, \tag{2}$$

where σ_{ij} is the stress tensor, D_i is the electric displacement vector and comma denotes spatial derivative. The constitutive equations reflecting fully-coupled piezoelectric effect can be expressed as

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} - e_{kij}E_k$$
$$D_i = e_{ikl}\varepsilon_{kl} + \epsilon_{ik}E_k, \tag{3}$$

in which ε_{kl} are strains, E_k are electric fields, C_{ijkl} are elastic constants, e_{kij} are piezoelectric constants and ϵ_{ik} are dielectric constants. Normally, hexagonal piezoelectric crystals exhibiting 6-mm symmetry will have x_3-axis as the c-axis with x_1-x_2 plane being isotropic. Here, in order to accommodate the spherical geometry of QD crystals, spherically–hexagonal anisotropy is assumed with the radial direction coinciding with the c-axis and θ and ϕ directions defining isotropic spherical surfaces. Then, the constitutive equations can be expressed in spherical coordinates with the R-direction coinciding with the c-axis,

$$\begin{pmatrix}\sigma_{RR}\\ \sigma_{\theta\theta}\\ \sigma_{\phi\phi}\\ \sigma_{\phi\theta}\\ \sigma_{\phi R}\\ \sigma_{\theta R}\end{pmatrix} = \begin{bmatrix} C_{33} & C_{13} & C_{13} & 0 & 0 & 0\\ C_{13} & C_{11} & C_{12} & 0 & 0 & 0\\ C_{13} & C_{12} & C_{11} & 0 & 0 & 0\\ 0 & 0 & 0 & (C_{11}-C_{12})/2 & 0 & 0\\ 0 & 0 & 0 & 0 & C_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & C_{44}\end{bmatrix} \times \begin{pmatrix}\varepsilon_{RR}\\ \varepsilon_{\theta\theta}\\ \varepsilon_{\phi\phi}\\ 2\varepsilon_{\phi\theta}\\ 2\varepsilon_{\phi R}\\ 2\varepsilon_{\theta R}\end{pmatrix} - \begin{bmatrix} e_{33} & 0 & 0\\ e_{31} & 0 & 0\\ e_{31} & 0 & 0\\ 0 & e_{15} & 0\\ 0 & 0 & e_{15}\\ 0 & 0 & 0\end{bmatrix}\begin{pmatrix}E_R\\ E_\theta\\ E_\phi\end{pmatrix}$$

$$\begin{pmatrix}D_R\\ D_\theta\\ D_\phi\end{pmatrix} = \begin{bmatrix} e_{33} & e_{31} & e_{31} & 0 & 0 & 0\\ 0 & 0 & 0 & e_{15} & 0 & 0\\ 0 & 0 & 0 & 0 & e_{15} & 0\end{bmatrix}\begin{pmatrix}\varepsilon_{RR}\\ \varepsilon_{\theta\theta}\\ \varepsilon_{\phi\phi}\\ 2\varepsilon_{\phi\theta}\\ 2\varepsilon_{\phi R}\\ 2\varepsilon_{\theta R}\end{pmatrix} + \begin{bmatrix}\epsilon_{33} & 0 & 0\\ 0 & \epsilon_{11} & 0\\ 0 & 0 & \epsilon_{11}\end{bmatrix}\begin{pmatrix}E_R\\ E_\theta\\ E_\phi\end{pmatrix}. \tag{4}$$

Likewise, the governing Eq. (2) in spherically symmetric coordinates can be expressed as

$$C_{33}u_{R,RR} + \frac{2}{R}C_{33}u_{R,R} + \frac{2}{R^2}(C_{13} - C_{11} - C_{12})u_R + e_{33}\Phi_{,RR} + \frac{2}{R}(e_{33} - e_{31})\Phi_{,R} = 0,$$
$$e_{33}u_{R,RR} + \frac{2}{R}(e_{33} + e_{31})u_{R,R} + \frac{2}{R^2}e_{31}u_R - \epsilon_{33}\Phi_{,RR} - \frac{2}{R}\epsilon_{33}\Phi_{,R} = 0. \tag{5}$$

The general solution for these electroelastically coupled differential equations can be obtained by the eigenvalue decomposition method as shown in the Appendix:

$$u_R = AR^{n_1} + BR^{n_2} + \frac{e_{31}C}{\gamma\beta\epsilon_{33}R},$$
$$\Phi = \left(\frac{e_{33}}{\epsilon_{33}} + \frac{2e_{31}}{\epsilon_{33}n_1}\right)AR^{n_1} + \left(\frac{e_{33}}{\epsilon_{33}} + \frac{2e_{31}}{\epsilon_{33}n_2}\right)BR^{n_2} + \left(\frac{e_{33}e_{31}}{\gamma\beta\epsilon_{33}^2} - \frac{2e_{31}^2}{\gamma\beta\epsilon_{33}^2} + \frac{1}{\epsilon_{33}}\right)\frac{C}{R} + F, \tag{6}$$