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Effect of Lattice Mismatch Strain Grading on the Electromechanical Behavior of Functionally Graded Quantum Dots

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Abstract. A fully coupled thermo-electro-mechanical models of cylindrical and truncated conical GaN/AlN Functionally Graded Quantum Dot (FGQD) systems with and without WL are analyzed in this study to determine the effect of lattice mismatch strain grading on the electromechanical behavior of the FGQD system. This has a technological and fundamental importance because the production methodology adopted for manufacturing QDs enables the composition of the QD material to be graded in the growth direction, so the material properties as well as the induced mismatch strain between the QD and the carrier matrix are accordingly graded. The power law is used to describe the grading function. Based on the obtained results, grading of material properties and lattice mismatch strain have significant effect on the distribution of the electromechanical quantities inside the QD and can be used as another tuning parameter in the design of QD systems.

Introduction

Due to their current and potential applications in optoelectronics, biotechnology and other areas, spatially confined motions of electrons in low dimensional semiconductor nanostructures (LDSNs), like quantum dots (QDs), have drawn increasing attention of physics and engineering communities [1]. LDSNs are strained structures as they are normally embedded in a host material with different structural properties. Piezoelectric effects in LDSNs are also important because most of the semiconductor materials are piezoelectric in nature [1]. Strain, piezoelectric and thermal effects are being used as tuning parameters for the optical response of LDSNs in band gap engineering.

In [2], [3], it was found that the production methodology adopted for manufacturing functionally graded QDs enables the composition of the QD material to be graded. This affects both the material properties as well as the initial strain induced in the QDs due to mismatch in lattice parameters of the QD and the carrier matrix. Patil and Melnik [1] presented a coupled model of thermo-electro-elasticity that was applied to the analysis of uniform QDs under different thermal loadings and their effects on the electromechanical properties and band structure of the QDs. Shodja and Rashidinejad [4] conducted a study on interacting functionally graded quantum wires (QWRs)/ QDs with arbitrary shapes and general anisotropy within a distinct piezoelectric matrix using an electromechanical equivalent inclusion method in Fourier space (FEMEIM). This study claimed the method to be able to readily treat cases where the QWRs/QDs are multiphase or functionally graded. However, it essentially focused on determination of two-dimensional electro-elastic fields of periodically as well as arbitrarily distributed interacting QWRs and QDs of arbitrary shapes within a piezoelectric matrix.

In the analysis of Pearson and Faux [5], dots with graded composition exhibited smaller strains at the base because the mismatch strain is lower at the base for this case, compared to dots with uniform composition. Several works have resolved strain distribution in different shapes via numerical methods. For example, Shin *et al.* [6] used the finite element method and analyzed structures similar to those in [5]. They reported the change in strain distribution with change in dot truncation as a function of stacking period.

Closed-form solutions were recently developed for QDs with graded eigenstrain in piezoelectric matrix. For example, exact closed-form solutions for an arbitrarily shaped polygonal inclusion with linearly [7] and quadratically [8] graded eigenstrain in an anisotropic piezoelectric half plane were developed. These analytical solutions assumed uniform material properties to simplify the formulation. A finite element model of a FGQD with both graded material properties and eigenstrain described by the power law (fractional exponents) in a piezoelectric matrix has not been investigated yet. This paper presents a fully coupled model of FGQD with functionally graded material properties and lattice mismatch strain in a host piezoelectric material. The grading is only applied in the thickness direction. The effects of the material property ratio, mismatch strain ratio and the power law index of the grading function on the electromechanical variables in the QD system are analyzed.

Governing Equations

The linear governing equations of thermo-electro-elasticity for a structure occupying volume Ω, under steady state conditions are the balance of linear momentum, Gauss's law for electrostatics, and the stationary heat conduction equation:

$$\sigma_{ij,j} + f_i = 0; \qquad D_{i,i} + q = 0; \qquad h_{i.i} - k = 0 \tag{1}$$

where σ_{ij}, D_i, h_i are the components of the stress tensor, electric displacement vector, and heat flux vector, and f_i, q and k are the mechanical body force vector, electric charge and heat source in Ω, respectively. Coupling of equations (1) is implemented through constitutive equations.

Gradient equations are defined as:

$$\varepsilon_{kl} = \frac{1}{2}\left(u_{k,l} + u_{l,k}\right); \qquad E_k = -\phi_{,k}; \qquad Q_k = -\Theta_{,k} \tag{2}$$

where, ε_{kl}, E_k, Q_k, u_k, ϕ and Θ are the components of the strain tensor, electric field vector, temperature gradient vector, mechanical displacement vector, electric scalar potential and temperature change from the reference temperature T_0, respectively.

The constitutive relations relating thermo-electro-mechanical quantities are expressed as

$$\sigma_{ij} = c_{ijkl}\varepsilon_{ij}\varepsilon_{kl} + e_{ijk}E_k - \beta_{ij}\Theta; \quad D_i = e_{ikl}\varepsilon_{kl} + \in_{ik} E_k + p_i\Theta + P_i^{sp}; \quad S = \beta_{ij}\varepsilon_{ij} + p_iE_i + \alpha_T\Theta \tag{3}$$

where, c_{ijkl}, e_{ijk} and $\in_{ik}$ are the elastic moduli, piezoelectric coefficients, and dielectric constants, respectively. P_i^{sp} is the spontaneous polarization, p_i and β_{ij} are thermoelectric and thermomechanical coupling constants, respectively. S denotes entropy. To take into account the lattice mismatch, the strain tensor components in eq. (2) for cylindrical symmetry take the form:

$$\varepsilon_{rr} = \frac{\partial u_r}{\partial r} - \varepsilon_a^*; \qquad \varepsilon_{zz} = \frac{\partial u_z}{\partial z} - \varepsilon_c^*; \qquad \varepsilon_{\theta\theta} = \frac{u_r}{r} - \varepsilon_a^*; \qquad \varepsilon_{rz} = \frac{1}{2}\left(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r}\right) \tag{4}$$

with $\varepsilon_a^* = \dfrac{a_m - a_{QD}}{a_{QD}}$ and $\varepsilon_c^* = \dfrac{c_m - c_{QD}}{c_{QD}}$ inside the QD. Quantities a_m, c_m and a_{QD}, c_{QD} are the lattice constants of the matrix and the QD, respectively, while quantities, ε_a^*, ε_c^* are the local intrinsic strains (lattice mismatch) along the a and c directions, respectively. The directions a and c correspond to the shorter and longer dimensions of the unit cell of the Wurtzite (WZ) crystal, respectively. As the substrate is relatively large compared to the QD, we follow common practice to neglect lattice mismatch inside the matrix [1], [9]. Thermal equilibrium is assumed throughout the problem domain. Therefore, the temperature change becomes spatially independent, effectively leading to the determination of the solution of the heat conduction equation in eq. (1). However, these equations are still coupled via the constitutive eqs. (3).

The material properties for WZ structures as well as the geometry and boundary conditions in this study are axisymmetric (no angular dependence), hence all the thermal, electric and mechanical field solutions are axisymmetric as well. The original 3D problem can then be reduced in this case to a simpler 2D problem in the plane of the axis of cylindrical symmetry. The linearly independent elastic constants and piezoelectric constants in a crystal with WZ symmetry are given as

$$\begin{gathered} c_{1111}=c_{11},\quad c_{1122}=c_{12},\quad c_{1133}=c_{13},\quad c_{3333}=c_{33},\quad c_{2323}=c_{44},\quad c_{2121}=(c_{11}-c_{12})/2, \\ e_{311}=e_{31},\quad e_{333}=e_{33},\quad e_{113}=e_{15},\quad \beta_{11}=\beta_1,\ \beta_{33}=\beta_3,\quad \in_{11}=\in_1,\ \in_{33}=\in_3 \end{gathered} \tag{5}$$

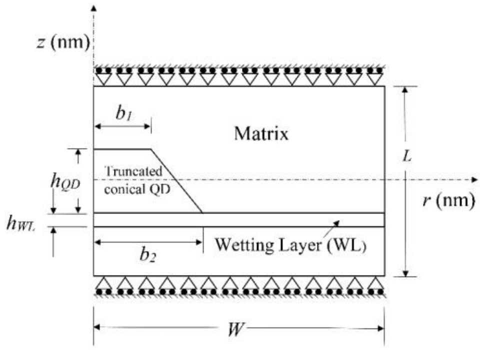
Grading function for material properties and lattice mismatch strain in a FGQD. All material properties in the QD will be graded as follows

$$P_{eff}(z)=P\left[1+\gamma\left(2f(z)-1\right)\right];\qquad \gamma=\frac{P_l-P_u}{P_l+P_u};\qquad f(z)=\left(0.5+\frac{z}{h_{QD}}\right)^n \mid z\in\left[-\frac{h_{QD}}{2},\frac{h_{QD}}{2}\right] \tag{6}$$

where $P_{eff}(z)$ is the effective material property of the FGQD; subscripts *u* and *l* denote, respectively, the upper and lower surface property of the FGQD. $P=P_{eff}(0)$ for linear grading (n = 1). When $n=0$, $P_{eff}=P_u=P(1+\gamma)$ and when $n=\infty$, $P_{eff}=P_l=P(1-\gamma)$ inside the QD.

Similarly, the effective mismatch strains of a functionally graded QD, in eq. (4), can be expressed as:

$$\varepsilon^*_{a_{eff}}(z)=\varepsilon^*_a\left[1+\rho\left(2f(z)-1\right)\right];\qquad \varepsilon^*_{c_{eff}}(z)=\varepsilon^*_c\left[1+\rho\left(2f(z)-1\right)\right];\qquad \rho=\frac{\varepsilon^*_{a_l}-\varepsilon^*_{a_u}}{\varepsilon^*_{a_l}+\varepsilon^*_{a_u}}=\frac{\varepsilon^*_{c_l}-\varepsilon^*_{c_u}}{\varepsilon^*_{c_l}+\varepsilon^*_{c_u}} \tag{7}$$



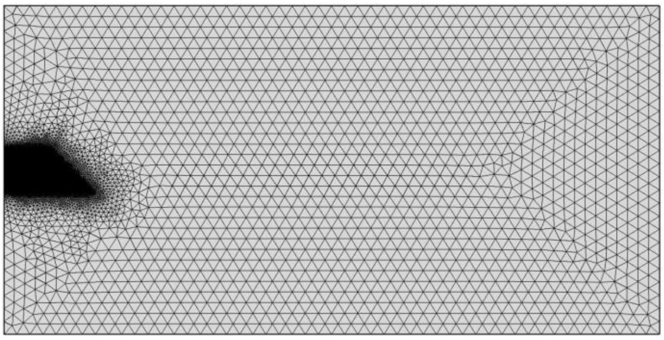


Fig. 1. (left) Geometry and co-ordinate system in (r, z) plane for a truncated conical QD with WL, (right) Finite element mesh of truncated conical QD without WL (axisymmetric model)

It should be noted that as n increases, larger portion of the QD will have values of mismatch strain closer to the values of mismatch strain at the base of the QD. This means smaller mismatch strains at the upper portion of the QD. In this work, we consider cylindrical and truncated conical QD geometry with and without wetting later (WL). Fig. **1** (left) shows the geometric details of the model. We use the following dimensions: height of the carrier matrix is L = 30 nm and its diameter $D = 2W$ = 120 nm, height of QD h_{QD} = 4 nm, upper and lower radii of the truncated conical QD b_1 = 4 nm and b_2 = 8 nm, and height of WL $h_{WL}=h_{QD}/4$ = 1 nm. Cylindrical QDs has constant radius b = 4 nm. The material properties of GaN/AlN QD system, which can be analyzed as a representative of III-V group semiconductors, are given in [10]. Based on the lattice constants, the values of lattice mismatch strain for GaN/AlN QD systems are: $\varepsilon^*_a=-2.47\%$ and $\varepsilon^*_c=-4.07\%$. The roller BCs for mechanical fields and Dirichlet condition for electric fields (electric ground) are imposed along the top and bottom faces of the system (see Fig. **1** (left)), the right face is traction free and electrically isolated, while symmetry boundary conditions are applied at the left face.

Finite Element model

A Finite Element Model (FEM) was developed in COMSOL Multiphysics using the Piezoelectric Devices (pzd) user interface, where initial stress ($\mathbf{S_0}$), initial strain ($\boldsymbol{\varepsilon}_\mathbf{0}$), and remanent electric displacement $\mathbf{D_r}$ can be defined. he stress-charge formulation of the constitutive relation for piezoelectric material with these initial fields are expressed as:

$$\mathbf{S}-\mathbf{S_0}=\mathbf{c_E}(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}_\mathbf{0})-\mathbf{e}^T\mathbf{E}; \qquad \mathbf{D}-\mathbf{D_r}=\mathbf{e}(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}_\mathbf{0})+\boldsymbol{\varepsilon}_\mathbf{S}\mathbf{E} \tag{8}$$

Here, $\boldsymbol{\varepsilon}$ is the strain, $\mathbf{S}$ is the stress, $\mathbf{E}$ is the electric field, and $\mathbf{D}$ is the electric displacement field. The material properties, $\mathbf{c_E}$, $\mathbf{e}$, and $\boldsymbol{\varepsilon}_\mathbf{S}$ correspond to the material stiffness tensor, piezoelectric coupling coefficients tensor, written in matrix form, and the electric permittivity matrix. Initial stresses in the QD and its carrier matrix are functions of stress-temperature coefficients for the corresponding material, while the initial strains in the QD correspond to the values of effective lattice mismatch strains for the whole system. The initial strain in the carrier matrix is assumed zero. The initial strain and stress tensors and the remanent electric displacement vector in GaN QD take the form:

$$\boldsymbol{\varepsilon}_\mathbf{0}=\begin{bmatrix}-\varepsilon^*_{a_{eff}}(z) & 0 & 0\\ 0 & -\varepsilon^*_{a_{eff}}(z) & 0\\ 0 & 0 & -\varepsilon^*_{c_{eff}}(z)\end{bmatrix}; \quad \mathbf{S_0}=\begin{pmatrix}-\beta_1(z) & 0 & 0\\ 0 & -\beta_1(z) & 0\\ 0 & 0 & -\beta_3(z)\end{pmatrix}T; \quad \mathbf{D_r}=\begin{pmatrix}0\\ 0\\ p_3(z)T+P^{sp}(z)\end{pmatrix}, \tag{9}$$

where T is the temperature. $\beta_1(z)$, $\beta_3(z)$, $p_3(z)$ and $P^{sp}(z)$ are graded in the GaN QD according to eq. (6), and uniform in the AlN host matrix. Convergent solution with smooth and accurate distributions of the electromechanical quantities along the axis of symmetry (r = 0) was achieved for the truncated conical QD without WL using 12,366 higher order triangular elements with "extra fine" mesh in the matrix domain (max. element size m = 1.2 nm) that is refined as we approach the domain of the QD where m = 0.1 nm, as can be seen in Fig. **1** (right).

Results

The results of the ungraded case are in very good agreement with the results in [1] and [9]. Figure 2 shows the effect of the material property ratio and lattice mismatch strain ratio on the z-component of electric field, the radial and transverse strain components of a truncated FGQD system without WL. We assume a constant temperature of 300 K and linear grading (n = 1). The case of ($\gamma = \rho = 0$) corresponds to ungraded structure and is added to facilitate the comparison. It can be observed that as γ increases, indicating increased intensity of material parameters in the growth direction, or ρ decreases, indicating decreased lattice mismatch strain in the growth direction, $|E_z|$ increases at the base of the FGQD and decreases at its top. So the case (ρ = -1/3; γ = 1/3) gave the maximum $|E_z|$ at the base of the QD, and the minimum at the top. The effect of ρ is much more significant on ε_{rr} than γ. As ρ decreases, $|\varepsilon_{rr}|$ increases at the base of the FGQD and decreases at its top. It is interesting to note that the significance of ρ and γ on ε_{zz} are of about the same order. Increasing γ or ρ will result in higher $|\varepsilon_{zz}|$ at the base of the FGQD and lower at the top. The case ($\rho = \gamma$ = 1/3) maximizes $|\varepsilon_{zz}|$ at the base of the QD. This case also resulted in tensile, rather than compressive, ε_{zz} at the top of the QD. The opposite case ($\rho = \gamma$ = -1/3) has opposite effects. Grading proved to be another effective tuning parameter that significantly alters the distributions of electromechanical fields in QD systems.

Fig. **3** shows the effect of power law index (n) on the electric potential and strain components along the z-axis at $r=0$ in the truncated conical GaN/AlN FGQD with ρ = -1/3; γ = 1/3 and T = 300 K. It can be observed that as n increases, the electric potential difference across the thickness of the FGQD ($\Delta\phi$), $|\varepsilon_{rr}|$ at the center of the QD, and $|\varepsilon_{zz}|$ inside the QD and in the host matrix increase.

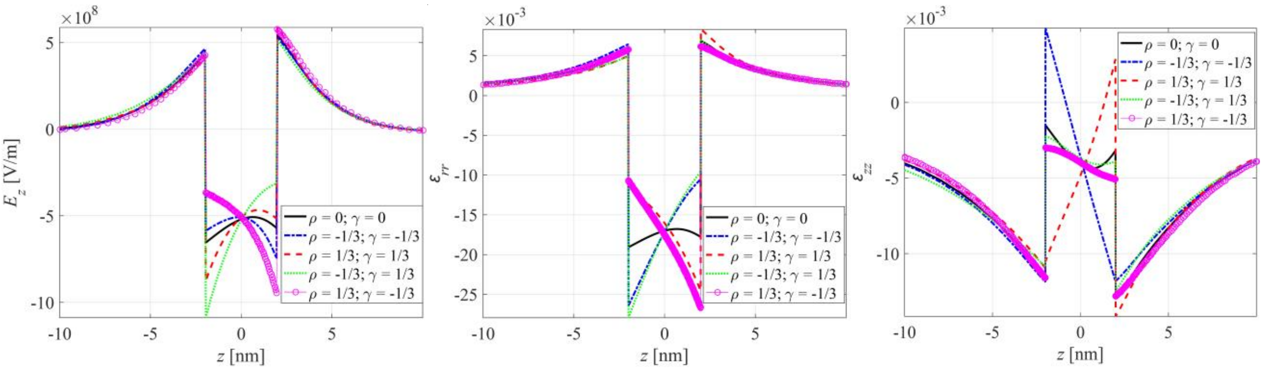


Fig. 2. Effect of initial lattice mismatch strain ratio ρ and material property ratio γ on E_z, ε_{rr} and ε_{zz} in truncated conical GaN/AlN FGQD without WL for n = 1, T = 300 K.

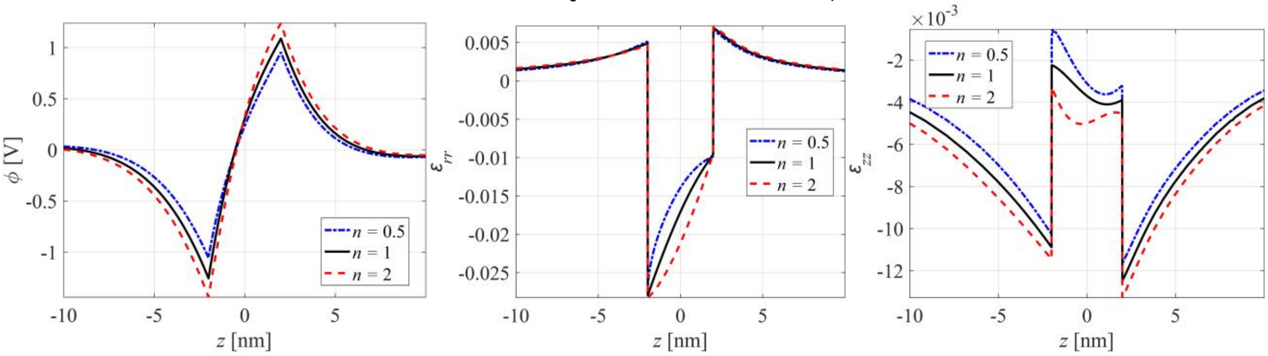


Fig. 3. Effect of power law index (n) and material property ratio γ on ϕ, ε_{rr} and ε_{zz} in truncated conical GaN/AlN FGQD without WL for ρ = -1/3; γ = 1/3, T = 300 K.

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