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Defects-enhanced flexoelectricity in nanostructures

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Abstract

Recent studies show that low dimensional nanostructures may exhibit nonlocal electromechanical effects such as flexoelectricity. Despite the recent progress in nanostructure growth techniques imperfections such as defects are practically unavoidable. These imperfections may enhance flexoelectric effects. Therefore, the main goal of this paper is to analyze the effects of these imperfections on linear electromechanical properties and on flexoelectricity. The constitutive relations for the adiabatically insulated reversible system are derived from the total differential of the general thermodynamic Gibbs potential. The mechanical and electrical balance equations coupled through the constitutive equations are then solved with finite element method for the defective nanostructures. We focus in our study on GaN-based nanostructures which are important in electronic and optoelectronic applications. They exhibit higher magnitudes of electric field compared to other semiconductors in similar contexts. Our results are presented for GaN quantum dots embedded in an AlN matrix.

Kyewords: Flexoelectrocity, defects, nanostructures

1. Introduction

In studying electronic and optoelectronic properties of low dimensional nanostructures for current and future applications, the linear electromechanical effects become increasingly important [1, 2, 3]. However, recent studies [1, 2, 4] show that these nanostructures also exhibit nonlinear electromechanical effects such as electrostriction [1] and nonlocal effects such as flexoelectricity [2]. Despite the universality of these phenomena in dielectrics, including centrosymmetric crystals, very little attention has been given to these effects in the context of nanostructures [2].

Lattice mismatch induced linear electromechanical effects in nano-heterostructures are now better understood [3]. At the same time, the interest to the nonlinear electromechanical effects has been growing continuously over recent years due to their importance in hetero-epitaxy grown nanostructures and other applications [5]. The recent progress in nanostructure growth techniques allows us to fabricate excellent nanostructures. Nevertheless, some imperfections such as defects are practically unavoidable. It is these imperfections that may lead to significant nonlocal electromechanical effects (in addition to lattice mismatch) such as flexoelectricity. Lattice mismatched nanostructures, such as GaN-based quantum dots (QDs) operating in high internal electric fields, of the order of 10^8

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V/m, may exhibit significant influence of these nonlinear and nonlocal effects on their electronic and optoelectronic properties [1, 3, 4]. This fact provides a major motivation for the current study of the role of nonlinear and nonlocal effects in GaN-based nanostructures and, in particular, in QDs. While in [1] a major focus was given to electrostriction, in this contribution our main attention is given to flexoelectric effects.

Nomenclature

σ_{ij}	stress tensor	D_i	electric displacement
f_i	body mechanical force	q	electric charge
ε_{kl}	strain tensor	E_n	electric field vector.
G_{ijkl}	flexoelectric coefficient	V	electric potential

2. Theory

We consider cylindrical QDs which are axisymmetric around z-axis (geometric details of which are given in Fig. 1). Governing equations for wurtzite (WZ) structures are axisymmetric, hence the solution of the model is axisymmetric as well. The material constants for the crystal with WZ symmetry used in this work are given in [3]. The original three-dimensional problem can be reduced in to a simpler two-dimensional problem by assuming axisymmetry along z-axis. The electromechanical balance equations in this case take the following form [6]:

$$\frac{\partial \boldsymbol{\sigma}_{rr}}{\partial \boldsymbol{r}} + \frac{\partial \boldsymbol{\sigma}_{rz}}{\partial z} + \frac{\boldsymbol{\sigma}_{rr} - \boldsymbol{\sigma}_{\theta\theta}}{\boldsymbol{r}} = \mathbf{0}, \quad \frac{\partial \boldsymbol{\sigma}_{rz}}{\partial \boldsymbol{r}} + \frac{\partial \boldsymbol{\sigma}_{zz}}{\partial z} + \frac{\boldsymbol{\sigma}_{rz}}{\boldsymbol{r}} = \mathbf{0}, \quad \frac{\partial \boldsymbol{D}_r}{\partial \boldsymbol{r}} + \frac{\partial \boldsymbol{D}_z}{\partial z} + \frac{\boldsymbol{D}_r}{\boldsymbol{r}} = \mathbf{0}. \tag{5}$$

These equations are invariant with respect to rotations around the z-axis, e.g. [3], hence solutions can be separated into a (r, z) part and a θ part, subject to adequate boundary conditions. The constitutive relations then take the following form for WZ nanostructures:

$$\begin{aligned}
&\boldsymbol{\sigma}_{rr} = \boldsymbol{C}_{11}\boldsymbol{\varepsilon}_{rr} + \boldsymbol{C}_{12}\boldsymbol{\varepsilon}_{\theta\theta} + \boldsymbol{C}_{11}\boldsymbol{\varepsilon}_{zz} - \boldsymbol{e}_{31}\boldsymbol{E}_z, \quad \boldsymbol{\sigma}_{rz} = \boldsymbol{C}_{44}\boldsymbol{\varepsilon}_{rz} - \boldsymbol{e}_{15}\boldsymbol{E}_r, \\
&\boldsymbol{\sigma}_{zz} = \boldsymbol{C}_{13}\boldsymbol{\varepsilon}_{rr} + \boldsymbol{C}_{13}\boldsymbol{\varepsilon}_{\theta\theta} + \boldsymbol{C}_{33}\boldsymbol{\varepsilon}_{zz} - \boldsymbol{e}_{33}\boldsymbol{E}_z, \quad \boldsymbol{D}_r = \boldsymbol{e}_{15}\boldsymbol{\varepsilon}_{rz} - \in_{11} \boldsymbol{E}_r \\
&\boldsymbol{D}_z = \boldsymbol{e}_{31}\boldsymbol{\varepsilon}_{rr} + \boldsymbol{e}_{31}\boldsymbol{\varepsilon}_{\theta\theta} + \boldsymbol{e}_{33}\boldsymbol{\varepsilon}_{zz} - \in_{33} \boldsymbol{E}_z + \boldsymbol{G}_{133}\boldsymbol{\varepsilon}_{zz,z} + \boldsymbol{P}_z^{SP}.
\end{aligned} \tag{6}$$

Note that based on the total differential of the general thermodynamic potential with Taylor series expansion of differentials of electromechanical quantities a generalization of Eq. (6) to the nonlinear case can be derived [3, 7]. To take into account the lattice mismatch, the strain tensor components take the following form:

$$\boldsymbol{\varepsilon}_{rr} = \frac{\partial \boldsymbol{u}_r}{\partial \boldsymbol{r}} - \boldsymbol{\varepsilon}_a, \quad \boldsymbol{\varepsilon}_{zz} = \frac{\partial \boldsymbol{u}_z}{\partial z} - \boldsymbol{\varepsilon}_c \quad \boldsymbol{\varepsilon}_{rr} = \frac{\boldsymbol{u}_r}{\boldsymbol{r}} - \boldsymbol{\varepsilon}_a, \quad \boldsymbol{\varepsilon}_{rz} = \frac{\mathbf{1}}{\mathbf{2}}\left(\frac{\partial \boldsymbol{u}_z}{\partial \boldsymbol{r}} + \frac{\partial \boldsymbol{u}_r}{\partial z} \right) \tag{7}$$

with $\varepsilon_a=(a_m-a_{QD})/a_{QD}$ and $\varepsilon_c=(c_m-c_{QD})/c_{QD}$ inside the QD. Quantities a_m, c_m and a_{QD}, c_{QD} are the lattice constants of the matrix and the QD, respectively [3, 5].

3. Results and Discussion

We discus here our results for WZ GaN/AlN QD systems, as a representative example, geometric details of which are given in Fig. 1. First, we discuss our results for the defects free GaN/AlN QD system with and without flexoelectricity. Next, we analyze the situation where the defects are located along the circumference of the cylindrical QD and then we study their effects on flexoelectricity. The defects are assumed to be introduced during the growth process. More precisely, we assume that some clusters of $Al_xGa_{1-x}N$ are present in the QD system, as it is often the case while growing QDs on different substrates [2, 5]. The extreme situation can be the presence of AlN clusters in the GaN QD. For our analysis we consider this extreme situation. We further assume that these AlN

clusters act as defects which are of elliptic shape with semi-major axis diameter of 0.4 nm and semi minor axis diameter of 0.1 nm. The results reported here are given for the situation where three such defects distributed along the circumference of the QD (z=0). More specifically we discuss our results for the following 6 different cases,

Case 1: Without defects, G_{133}=0.0 C/m
Case 2: Without defects, G_{133}=1×10^{9} C/m
Case 3: With defects, G_{133}=0.0 C/m
Case 4: With defects, G_{133}=1×10^{-10} C/m
Case 5: With defects, G_{133}=5×10^{-10} C/m
Case 6: With defects, G_{133}=1×10^{-9} C/m.

The model based on Eqs. (5-7) is solved numerically with finite element method and the details of boundary conditions and the numerical procedure applied here can be found in [3].

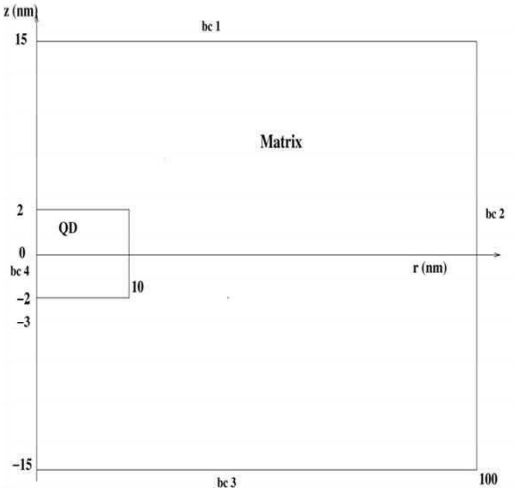


Fig. 1 Geometry of the GaN/AlN QDs

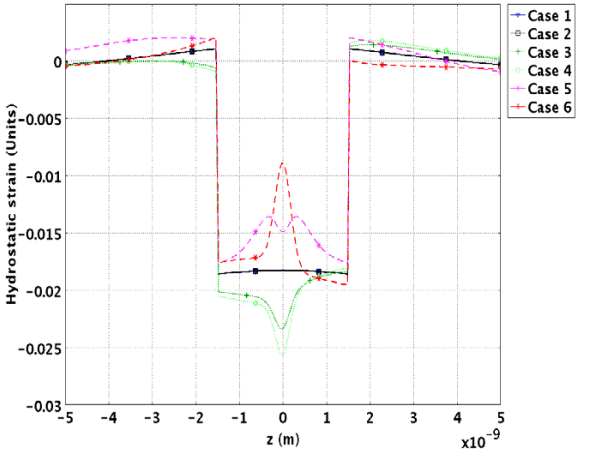


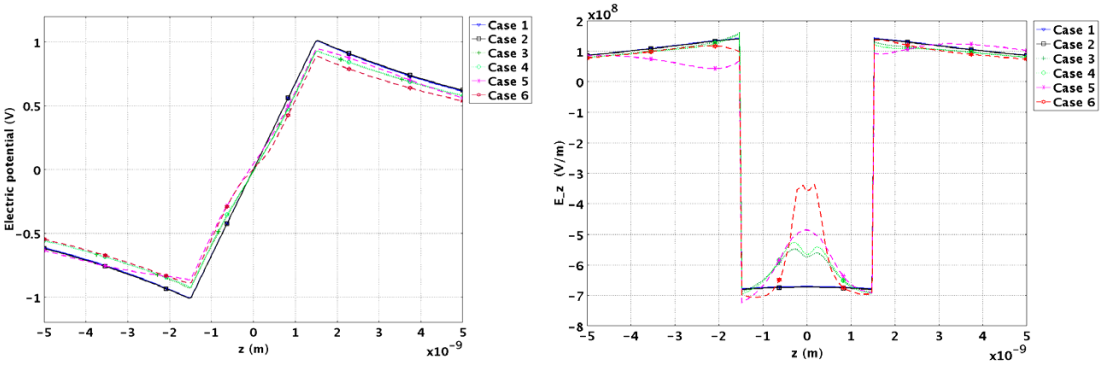
Fig. 2.Effect of flexoelectric coefficient on hydrostatic strain in the defect free and defective GaN/AlN QDs

Figure 2 shows the hydrostatic strain along the *z*-axis for the defective and defect free GaN/AlN QD system, with and without flexoelectric effect. In the defect free case (Case 1), accounting for flexoelectricity (Case 2) does not change the hydrostatic strain inside or outside the QD. Similar observations are made for the electric potential and electric field. This is due to a relatively small magnitude of the strain gradient on which flexoelectricity depends. However, one can expect higher strain gradients in the case of defective QDs. Indeed, the strain profile changes significantly with the flexoelectric coefficient. The magnitude of the hydrostatic strain decreases with the increase in the flexoelectric coefficients (Case 3 to Case 6).

Figure 3 shows the electric potential and the *z*-component of the electric field along the *z*-axis for the defective and defect free GaN/AlN QD system, with and without flexoelectric effect. The highest magnitude (~2V) of the electric potential is observed in the case of defect free QDs (Case 1 and 2). On introducing defects (Case 3 to Case 6), the electric potential decreases to ~1.7 V (Fig. 3a). Furthermore, as the value of the flexoelectric coefficient increases, the electric potential along with the hydrostatic strain (Fig. 2) decrease due to the additional degrees of freedom available for misfit strain relaxation. The lowest magnitude of potential difference across the top and bottom of the QD is ~1.6 V. The decrease of 40 mV in the electric potential is attributed to the introduced defects and the flexoelectric effect. It should also be noted that the potential curve becomes smoother with increasing flexoelectric coefficient, which may lead to lower values of the internal electric field. The *z*-component of the

electric field decreases with the introduction of defects and with increasing flexoelectric effect (Fig. 3b). The change in the internal electric field becomes more significant at higher values of the flexoelectric coefficient. The magnitude of the electric field varies from ~7×10^8 V/m for the defect free case to ~3.5×10^8 V/m for the defective QD with highest magnitude of the flexoelectric coefficient.

The magnitudes of the electromechanical parameter are in good agreement with corresponding cases from previous studies [1, 3, 6]. The flexoelectric effect can be significant in the defective nanostructures as it leads to irregular strain profiles, which may lead to higher magnitudes of the strain gradients. The defects and impurities are often present in the nanostructures due to higher surface to volume ratio, dangling bonds and the growth process [2, 5]. Hence, the significant influence of the flexoelectric effect can be expected on the electromechanical properties of the nanostructures and subsequently on their optoelectronic properties [3].



a) Electric potential b) z-component of electric field

Fig. 3 Effect of flexoelectric coefficient on electric field and potential in the defect free and defective GaN/AlN QDs

4. Conclusions

The nonlocal effects such as flexoelectricity are more prominent when defects in the nanostructures taken into account due to the appearance of higher strain gradients. Linear electromechanical properties are also significantly altered due to flexoelectricity and associated defects. The hydrostatic strain value decreases with increase in the flexoelectric coefficient. The electric potential variation becomes smoother due to the flexoelectric effect which leads to lower values of the internal electric field.

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