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Thermopiezoelectric and Nonlinear Electromechanical Effects in Quantum Dots and Nanowires

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Abstract. We report thermopiezoelectric (TPE) and nonlinear electromechanical (NEM) effects in quantum dots (QD) and nanowires (NW) analyzed with a model based on coupled thermal, electric and mechanical balance equations. Several representative examples of low dimensional semiconductor structures (LDSNs) are studied. We focus mainly on GaN/AlN QDs and CdTe/ZnTe NWs which we analyze for different geometries. GaN/AlN nano systems are observed to be more sensitive to thermopiezoelectric effects than those of CdTe/ZnTe. Furthermore, noticeable qualitative and quantitative variations in electromechanical fields are observed as a consequence of taking into account NEM effects, in particular in GaN/AlN QDs.

Keywords: Quantum Dots, Nanowires, Thermopiezoelectric, Nonlinear Electromechanical Effects
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INTRODUCTION

Strained LDSNs often exhibit piezoelectricity as most of the semiconductor materials are piezoelectric in nature. Strain and piezoelectric effects may contribute significantly to the overall properties of these structures [1]. In addition, thermal effects are becoming increasingly important as novel LDSN-based electronic/optoelectronic devices face challenges in thermal management. It is expected however, that by integrating LDSN materials into critical regions of microelectronic circuit, the excess heat that limits device performance can be effectively removed [2]. Nevertheless, a combined influence of thermal and electromechanical fields remains to be clarified. Indeed, recently it has been shown that the conventional application of linear models to the analysis of opto-electro-mechanical properties of nanostructures in band structure engineering could be inadequate and accounting for nonlinear strain effects in the full 3D models for nanostructures may be required [3]. Therefore a more systematic study on thermal loadings is required to analyze and optimize their effect on optoelectronic properties of LDSNs.

In this contribution, we report the study of TPE and EM effects in QDs and NWs based on a coupled 3D model. A major focus is given to the study on GaN/AlN QDs and CdTe/ZnTe NWs with different geometries.

THEORY

In order to study TPE and and EM effects in QDs and NWs we formulate a mathematical model accounting for these effects. The problem is governed by a coupled system of equations of elasticity and electrostatics.

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

$$D_{i,i} - q = 0, \tag{2}$$

where σ_{ij} are stress tensor components, D_i are electric displacement vector components, f_i and q are body mechanical forces and electric charge, respectively. The constitutive equations that account for TPE and EM effects are [4]

$$\begin{aligned} \sigma_{ij} &= c_{ijlm}\varepsilon_{lm} - e_{ijn}E_n + \frac{1}{2}c_{ijlmpq}\varepsilon_{lm}\varepsilon_{pq} && (3)\\ &\quad -\frac{1}{2}B_{ijnr}E - nE_r - \gamma_{ijlmn}\varepsilon_{lm}E_n - \beta_{ij}T, \\ D_k &= e_{klm}\varepsilon_{lm} + \varepsilon_{kn}E_n + \frac{1}{2}\gamma_{klmpq}\varepsilon_{lm}\varepsilon_{pq} && (4)\\ &\quad +\frac{1}{2}\varepsilon_{knr}E_nE_r + B_{klmn}\varepsilon_{lm}E_n + P^{sp} + p_kT, \end{aligned}$$

where σ, ε, E_n and D_k are stress, strain, electric field and electric displacement respectively, $c, e, \gamma, \varepsilon, \beta, p$ and B are compliance, piezoelectric, nonlinear piezoelectric, nonlinear dielectric permittivity, stress-temperature, pyroelectric and electrocstriction coefficients respectively and P^{sp} is the spontaneous polarization.

RESULTS

Magnitudes of the electromechanical quantities at the center of the QDs and NWs are tabulated in Table 1.

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TABLE 1. Magnitudes of electromechanical quantities at the center of the QDs and NWs

	CdTe/ZnTe*		GaN/AlN†(TC)**	
	0K	1000K	0K	1000K
$\varepsilon_{rr}(\%)$	4.3	4.5	0.65(1.05)	0.4(0.8)
$\varepsilon_{zz}(\%)$	4.4	4.5	0.18(0.15)	0.47(0.5)
V(V)	0.78	0.76	2.45(3.4)	2.2(3.0)
E_z(MV/cm)	0.1	0.1	6.0(6.7)	5.0(5.8)

* Rectangular box shaped NW, $10 \times 10 \times 70$ nm
† Cylindrical QD without wetting layer (WL), radius 4 nm and height of 4 nm
** TC, Truncated conical QD with WL (thickness = 1 nm), top radius 4 nm, bottom radius 8 nm and height of 4 nm.

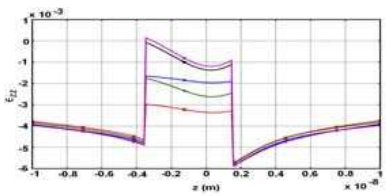

FIGURE 1. Strain in z-direction (ε_{zz}). Linear case: line-star, nonlinear case: $M_{33} = 10^{-18}(m^2/V^2)$[6] (line-triangle), $10^{-19}[m^2/V^2]$ (line-square), $10^{-20}[m^2/V^2]$ (line-plus) and $10^{-21}[m^2/V^2]$ (line-circle)

GaN/AlN QD systems are more sensitive to temperature compared to CdTe/ZnTe NWs, due to the low values of stress-temperature coefficients and relatively weak piezoelectric coupling. The physical parameters, for computations carried out here have been as in [1, 5]. A giant built-in electric field of several MV/cm is the characteristic of GaN/AlN structures and has been observed in several experiments, which agrees well with our results (6-8 MV/cm) [1]. Maximum magnitude of strain tensor component, ~4.5% (~1.0%) is observed near the edges of the CdTe/ZnTe NWs (GaN/AlN QDs). The potential difference across the CdTe/ZnTe NW ends is ~0.08 V, which is smaller than GaN/AlN QD (~2V) by order of magnitudes. The magnitude of the electric field in CdTe/ZnTe NW is in fractions of MV/cm, which is very small as compared to that of in GaN/AlN QD (~6 MV/cm).

Figures 1 and 2 show ε_{zz} in z-direction as a function of choice of B_{333} and effect of nonlinearity on electric potential in truncated conical GaN/AlN QD, respectively. We use a range of values for B_{333} since experimentally obtained value is relatively high compare to the materials in the same group [6]. ε_{zz} oscillates between ~-0.8% to ~-3.4% with increase in B_{333}. It can be seen that ε_{zz} changes to a flat line as electrostrictive coefficient increases as electric potential decreases due to dominating

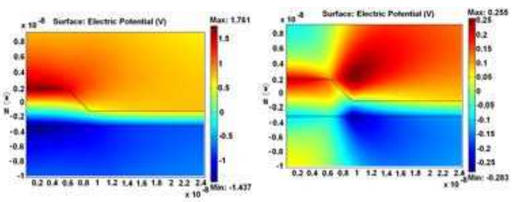

FIGURE 2. Surface view of electric potential

nonlinear effect. The maximum and minimum voltages have dropped dramatically from ~1.761 V to ~0.255 V and from ~-1.437 V to ~-0.283 V due to the incorporation of higher order effects (Fig. 2).

CONCLUSIONS

The strongly coupled TEM 3D calculations have been performed for GaN/AlN QDs and CdTe/ZnTe NWs with different geometries along with WL. The GaN/AlN QD systems show order of magnitudes higher electric quantities than that of CdTe/ZnTe NWs and is more sensitive to thermal loadings. CdTe/ZnTe based LDSNs may have an advantage in generating optical gain over GaN based LDSNs as they have smaller magnitudes of internal electric field and negligible spontaneous polarization. The effects of the electrostriction have been investigated by comparing various electrostriction coefficients and noticeable changes are observed in electric quantities.

ACKNOWLEDGMENTS

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