



Coupled Magneto-Thermo-Electromechanical Effects and Electronic Properties of Quantum Dots

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For the first time, we systemically analyze the influence of magneto-thermo-electromechanical effects on the band structure calculations by using the fully coupled model. We focus on three different types of quantum dots (QDs): (a) ferroelectric, (b) piezomagnetic, and (c) magnetoelectric, with and without wetting layers (WLs). We demonstrate that the influence of such coupled effects in the general fully coupled framework for studying properties of QDs can be significant and we quantify these effects in each case. For example, in magnetic GaN/BaTiO₃ QDs, we found that the influence of electromechanical effects on the band structure calculations and the spin splitting energy are practically independent of temperature. However, in piezoelectric AlN/GaN QDs, the influence of temperature on the electromechanical effects, electronic properties and spin splitting energy is significant. In particular, in piezoelectric AlN/GaN QDs, the intra-subband energy (i.e., the energy difference between ground and first excited states) decreases with the increase in temperature.

Delivered by Publishing Technology to: Universite de Montreal - Bibliothèques - Acquisition (PER)
Keywords: Quantum Dots, Coupled Magneto-Thermo-Electromechanical Effects, Ferroelectric, Piezoelectric, Magnetoelectric, Band Structure Calculation, Quantum Mechanics
07-Mar-2013
American Scientific Publishers

1. INTRODUCTION

It has been known that both strain and such fields as magnetic, thermal, electromechanical can be used as tuning parameters for the optical response of Low Dimensional Semiconductor Nanostructures (LDSNs) in photonics, band gap engineering, optoelectronics and other applications.¹⁻⁵ The combined influence of these fields in the magnetic QDs can lead to their significant contributions in band structures of LDSNs used at the device level (e.g., non-volatile memory devices).^{1,2} Furthermore, the investigation of the electron spin splitting energy due to spin-orbit interaction in QDs is also essential.⁶⁻⁹ These coupled multiphysics effects in properties of QDs grow into a substantial factor to be accounted for in many current and potential applications of optoelectronic devices, as well as in other applications.^{1,7,10-15}

Among LDSNs, wide band gap semiconductor nanostructures such as AlN/GaN QDs doped with magnetic materials (e.g., Mn or Cr), have attracted significant attention due to their current and potential applications in optical, optoelectronic and electronic devices used in

nano- and bionano-technological applications.¹⁶⁻¹⁹ Several other classes of LDSNs also present significant interest for applications. Indeed, ferroelectric nanostructures such as BaTiO₃ or PZT are important for the design of nonvolatile memory density devices, actuators and transducers, etc.²⁰⁻²⁴ The class of multiferroic nanostructures provides another important example for applications.^{4,25,26}

In these nanostructures, strain is induced due to the lattice mismatch at the interfaces of the heterojunction that can be used to design new promising devices such as spintronic.^{8,27-35} Although some coupled effects were included in the study of LDSNs (e.g., Refs. [10,29]), the influence of coupled magneto-thermo-electromechanical effects has not been studied systematically.

Another point to note is that the Rashba spin-orbit coupling can be used as a key parameter in controlling the electron spin in AlN/GaN QDs.^{8,36} The mathematical expression for the Rashba spin-orbit coupling (given later in this paper in Eq. (22)) is well established for semiconductor heterojunction-type devices.^{11,37} In several recent works, the Rashba spin-orbit coupling in QD systems was explored by several different groups (see Refs. [38–42]). However, the influence of the coupled magneto-thermo-electroelasticity in QDs has been largely neglected in the

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literature and we intend to cover this gap. In this context we mention Ref. [43] where the authors studied the electronic properties of AlGaIn/GaN/BaTiO₃ double heterostructures by combining first principles and charge control method. Our approach developed here is different from earlier studies (e.g., Ref. [43]). We investigate the influence of magneto-thermo-electromechanical effects on the ferroelectric, piezomagnetic and magnetoelectric QDs based on the fully coupled quantum-continuum models implemented via the finite element methodology.⁴⁴

Various approaches such as atomistic, pseudopotential, and tight binding have been applied to investigate the optical and electronic properties of LDSNs.^{45,48} In this paper, we apply the $k \cdot p$ methodology which allows us to incorporate electromechanical and other coupled effects in the band structure calculations of QDs in a straightforward manner.^{49,50}

In what follows, we undertake a systematic study of the coupled effects of magneto-thermo-electroelasticity in three different types of nanostructures: (a) ferroelectric (b) piezomagnetic (multiferroic, magnetostrictive) and (c) magnetoelectric. We also present a numerical analysis of these effects on the electronic properties of QDs.

The rest of the paper is organized as follows. In Section 2, we provide details of the models to account for the influence of electromechanical effects on the properties of wurtzite QD structures. We also provide their generalizations to the coupled magneto-thermo-electroelasticity. In Section 3, we give details of the total Hamiltonian $H = H_0 + H_{int}$ including classical and quantum parts. In Section 4, we present the developed mathematical models in cylindrical coordinates to study the magneto-thermo-electromechanical effects on the band structures of wurtzite QDs. Section 5 presents a series of numerical results demonstrating the influence of magneto-thermo-electromechanical effects on the properties of ferroelectric, piezomagnetic and magnetoelectric QDs. Finally, Section 6 summarizes our findings.

2. COUPLED EFFECTS IN QUANTUM DOTS

In this section, we provide details of a mathematical model to study the influence of magneto-thermo-electromechanical effects on the properties of wurtzite QD structures.

2.1. Balance Equations for Mechanical, Electric and Thermal Fields

Following Refs. [29,49,50], a coupled system of mechanical, electrostatics and thermal energy balance equations to study thermo-electromechanical effects in QDs with axial symmetry can be written as:

$$\sigma_{ij,j} + f_i = 0 \quad (1)$$

$$Dt.i \sim q = 0 \quad (2)$$

$$h_{i,t} - k = 0 \quad (3)$$

Here σ_{ij} are the stress tensor components, D_i are the electric displacement vector components and h_i are the heat flux vector components. Also, f_i are the components of body mechanical forces, q is the electric charge and k is the heat source. Constitutive equations for the system (1)-(3) in a more general setting are given below, in Section 2.3.

2.2. Gradient Equations

The equations that relate the linear strain (for generalization to nonlinear strain models, see Refs. [28,51-54]) and mechanical displacement, electric field and electric potential, the thermal field and temperature change, are referred to as gradient equations which can be written as,

$$\epsilon_{kl} \sim \frac{1}{2} (u_{k,l} + u_{l,k}) \quad (4)$$

$$E_k = -V_{,k} \quad (5)$$

$$\theta_k \sim -T_{,k} \quad (6)$$

$$Q_k \sim -\Theta_{,k} \quad (7)$$

where ϵ_{kl} are the strain tensor components, E_k is the electric field vector, Q_k is the thermal field vector, u is the mechanical displacement vector, V_k is the electric potential and $\Theta_{,k}$ is the change in temperature from the reference temperature Θ_0 .

2.3. Fully Coupled Magneto-Thermo-Electromechanical System

The coupled system of magneto-thermo-electroelasticity including the Navier and Maxwell's equations that account for the piezoelectric field⁵⁵ can be written as

$$\partial_j \sigma_{ik} = 0 \quad (8)$$

$$djDt = 0 \quad (9)$$

$$\partial_i H_i = 0 \quad (10)$$

$$\partial_i q_i = 0 \quad (H)$$

The components σ_{ij} , H_i and q_i are coupled via the Helmholtz free energy function:²⁹

$$\begin{aligned} \Phi(\epsilon_{ij}, E_i, \theta, B_p) &= \frac{1}{2} C_{ijkl} \epsilon_{ij} \epsilon_{kl} - \epsilon_{ijk} E_j B_k - \frac{1}{2} \epsilon_{ij} E_i E_j - \beta_{ij} \theta \epsilon_{ij} \\ &\sim P_i^E \epsilon_{ij} - \frac{1}{2} a_T \theta^2 + \frac{1}{2} p_{pq} B_p B_q + \frac{1}{2} p_{ij} \epsilon_{ij} B_p \\ &- X_{pm} E_m B_p - T_p B_p \end{aligned} \quad (12)$$

where $v_{pq} = i/p_{pq}$ and p_{pq} is the permeability coefficient, $i_{r_{pi}}$ is the piezo-magnetic coefficient, A_{pm} is the electromagnetic coefficient and T_p is the thermo-magnetic

coupling. Also $a_T = \epsilon_s^V / T_{DP}$ and is the heat capacity at constant strain tensor and at constant electric potential. The resulting constitutive equations in this case can be written as:

$$\sigma_{kl} = \left(\frac{d\epsilon_{kl}}{dt} \right)_{E,B,\Theta} = c_{ijkl} \epsilon_{ij} - e_{mkl} E_m - \pi_{pkl} B_p - \beta_{kl} \Theta \quad (13)$$

$$D_n = - \left(\frac{\partial \Phi}{\partial E_n} \right)_{\epsilon, B, \Theta} = e_{nij} \epsilon_{ij} + \epsilon_{mn} E_m + \lambda_{pn} B_p + p_n \Theta \quad (14)$$

$$H_q = \left(\frac{\partial \Phi}{\partial B_q} \right)_{\epsilon, E, \Theta} = -VqijSij - \epsilon_{mkl} E_m + \pi_{pkl} B_p + \beta_{kl} \Theta \quad (15)$$

$$s = (-) \left(\frac{\partial \Phi}{\partial \epsilon_{EB}} \right) = \beta_{ij} \epsilon_{ij} + P_n E_m + r_p B_p + a_T \Theta \quad (16)$$

where e_{ik} is the piezoelectric coefficient, ϵ_n is the permittivity, P_{sp} is the spontaneous polarization and E_m is the built in piezoelectric field. It is also well known that the internal strain reduces the band gap in semiconductor nanostructures, influencing the quantum confinement effect.⁵⁶ In what follows, we apply the Lifshits-Rozentsveig theory that accounts for the internal strain (Swfgytfe: 57, 58) Cauchy strain and the internal strain (Mliltf^Tili55j{thh: Thu, Q^tM3fs8Q^SiW&il^nter action is an essential ingred-

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$$\epsilon_{ij} = \epsilon_{ij}^0 + \epsilon_{ij}^1 \quad (17)$$

where ϵ_{ij}^0 are the local intrinsic strain tensor components due to lattice mismatch and ϵ_{ij}^1 are position dependent strain tensor components. These two can be written as

$$4 = (8_{ij} - 8^{\wedge}) < + 8^{\wedge} X \quad (18)$$

$$\epsilon_{ii} = \frac{1}{2} (\partial_j u_i + \partial_i u_j) \quad (19)$$

where $\epsilon_a^* = (a_m - a_{QD}/a_{QD})$ and $\epsilon_c^* = (c_m - c_{QD}/c_{QD})$ are the local intrinsic strains along a and c directions, respectively.⁵⁹ Also, a_m , c_m and a_{QD} , c_{QD} are the lattice constants of the matrix and the QD, respectively.

3. HAMILTONIANS OF QUANTUM DOTS ACCOUNTING FOR CLASSICAL AND QUANTUM PARTS

The band diagram calculation of self-assembled QDs requires a solution of the Schrödinger equation supplemented by a system of partial differential equations that account for coupled classical effects. In particular, for epitaxially grown self-assembled QDs in presence of externally applied electric fields, we need special care in the inclusion of electromechanical effects into the Hamiltonian of QDs.⁶⁰ In addition, applied magnetic fields must be

gauge invariant in the solution of Schrödinger equation to study the spin splitting energy of QDs.⁶¹ We calculate the electronic properties of QDs by using the relativistic $k \cdot p$ envelope function method that up to date has been successfully applied to include the influence of the magnetic⁶² and thermo-electromechanical fields²⁹ separately. The total Hamiltonian of the QDs in this case can be written as

$$H = H_{k,p}^{n \times n} + H_R + H_e^s \quad (20)$$

Here, H_R is the Rashba (Rashba-Bychkov) spin orbit interaction and H_e^s is the strain dependent part of the kinetic energy of the electron to be discussed later. The remaining portion of the Hamiltonian can be written as,

$$H_{k,p}^{n \times n} = p_x \frac{1}{m_e^*} p_x + p_y \frac{1}{m_e^*} p_y + p_z \frac{1}{m_e^*} p_z + E_c + \frac{1}{2} g_0 \mu_B B \sigma_z \quad (21)$$

where the kinetic momentum operator $\vec{P} = \vec{p} + e/c\vec{A}$ is the sum of the conical momentum operator $\vec{p} = -i\hbar(\partial_x, \partial_y, 0)$ and $\vec{A} = (B/2)(-y, x, 0)$ which is the vector potential in symmetric gauge. Here B is the applied magnetic field along z -direction, μ_B is the Bohr magneton, $E_c(r_0)$ is the conduction band edge profile and e is the electronic charge. We denote by σ , the usual Pauli spin matrix along z -direction. The strain dependent part of the electron Hamiltonian in (20) can be written as^{67,36,38}

$$H_R = a_R P_y \sigma_x - a_x P_x \sigma_y \quad (22)$$

where a_R is the Rashba coefficient for spin orbit interaction, a_x and a_y are the Pauli spin matrices along x and y -directions.

The strain dependent part of the electron Hamiltonian in (20) can be written as

$$H_e^s = a_c^{\parallel}(r) \epsilon_z(r) + a_c^{\perp}(r) \epsilon_{\perp}(r) + e_y(r) J \quad (23)$$

where ϵ_{zz} and ϵ_{\perp} are the conduction band deformation potentials along and perpendicular to the symmetric axis.

4. QUANTUM-CONTINUUM MODEL IN CYLINDRICAL COORDINATES AND ITS COMPUTATIONAL IMPLEMENTATION

Based on the coupled model described in Sections 2 and 3, in this section, a general two-dimensional (2D) model in cylindrical coordinates has been developed to study the influence of the magneto-thermo-electromechanical effects on the band structures of QDs having cylindrical symmetry. Examples that follow focus on wurtzite QDs. In this case, with appropriate boundary conditions, the solutions

to Eqs. (8)-(11) are also axisymmetric.^{29,63} Therefore, in this special case, the original 3D problem can be reduced to a 2D problem.⁶⁴ The linearly independent elastic constants and piezoelectric constants in a crystal with wurtzite symmetry are given as

$$\begin{aligned} \text{Cui!} - \text{C}_{1122} - \text{C}_{12}, & \quad \text{Cl } 133 = \text{C}_{13}, \\ \text{C}3333 - \text{C}33, & \quad \text{C}_{2323} = \text{C}44, \\ \text{C}2121 - 2^{n-1} \text{Cn} & \quad *311 = *31, \\ *333 - *33 & \quad *113 = *15, \\ 3n^7/3i, & \quad \wedge 33 - \wedge 3^2 \text{Cn} = \text{E}1, \quad \text{e}_3 = \text{E} \end{aligned}$$

The magneto-thermo-electromechanical balance equations in cylindrical coordinates for axially symmetric QDs of wurtzite structure can be written as (see e.g., Refs. [28,63,65])

$$\frac{\partial \sigma_{rr}}{dr dz} + \frac{\partial \sigma_{rz}}{\partial z} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0 \quad (24)$$

$$\frac{da_{r7}}{dr} + \frac{da_{zz}}{dz} + \frac{1}{r}\sigma_{r7} = 0 \quad (25)$$

$$\frac{dD}{dr} + \frac{dD}{dz} + D = 0 \quad (26)$$

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Copyright American Scientific Publishers, we have:⁴²

$$\frac{da}{dr} + \frac{da}{dz} + \frac{a}{r} = 0 \quad (28)$$

The stress tensor components, the electric displacement vector components, the magnetic field components and the heat fluxes are determined by the following constitutive relationships:

$$\begin{aligned} \sigma_{rr} = & C_1] \mathbf{f}_{rr} + C_n^{\ell} ee + C_{13} \mathbf{f}_{77} + d_{71} V \\ & + f_{11} \partial_r \phi - \beta_1 \Theta \end{aligned} \quad (29)$$

$${}^a_{ee} - C_{11} \mathbf{f}_{QQ} + C_{12} \mathbf{e}_{rr} + C_{13} \mathbf{f}_{77} - \mathbf{e}_{31} d_7 V + \frac{1}{31} d^{\wedge} - \mathbf{f}_{t0} \quad (30)$$

$$\langle V_Z = 2C_{44}\mathbf{f}_{r,7} + \mathbf{e}_{15}\mathbf{a}_r V - k f_{15} d_r \rangle \quad (31)$$

$$\sigma_{zz} = C_{13}e_{rr} + c_{13}\epsilon_{00} + c_{17}\epsilon_{77} + t_{33}a_{,v} + \frac{1}{33}d^{ftO} \quad (32)$$

$$D_{\alpha} = 2e_{15}f_{r7} - e_{11}a_r V - g_{11}d_r^{\wedge} \quad (33)$$

$$\begin{aligned} \Lambda_Z = & *31 \left({}^e\text{rr} \text{ "I" } {}^e\text{ee} \right) {}^e33{}^e??. \sim {}^e3\Lambda_Z^V \\ & + P_z^{sp} - g_{33} \partial_z \phi + \tau_3 \Theta \end{aligned} \quad (34)$$

$$B_r = 2/5 e_{rz} - g_{11} d V - Mn^{</>} \quad (35)$$

$${}^5Z = Al(e_{rr} + e_{ee}) + 33e_{zz} - M33a_z / \sqrt{P30} \quad g_{33} \partial_z V \quad (36)$$

$$q_r = -\lambda_1 A \quad (37)$$

$$q_7 = -k_{33}d_7^{\textcircled{\text{R}}} \quad (38)$$

where, as before, c_{ij} are the elastic moduli, e_{ij} are the piezoelectric coefficients, ϵ_{ij} are the permittivities, V is the (piezo) electric potential and $E_m = -dV/dz$ is the built in (piezo)electric field. Also, μ_{ij} is the permeability, $B = -dc_f/dz$ is the magnetic induction and ϕ is the magnetic potential, f_α , r_h , p - and O are the thermal stress, pyroelectric, pyromagnetic coefficients and temperature gradient from the reference point respectively, q_s is the heat flow and k_{ij} is the heat induction coefficient. We consider the temperature as an external parameter (for the analysis of thermo-electromechanical coupling, we refer to Ref. [29] for more details). Therefore, Eqs. (28), (37) and (38) are satisfied automatically in our wurtzite quantum dot nanostructures.

In our case we have

$$\sigma_{rr} = \frac{dU_r^*}{dr} + \varepsilon_a, \quad \varepsilon_{zz} = \frac{dw}{dz} + \varepsilon_c \quad (39)$$

$$\mathbf{f}_{ee} = - + \frac{v_r}{r} \mathbf{f}_r \quad \star \quad \mathbf{z} = \frac{1}{2} \left(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r} \right) \quad (40)$$

The Rashba spin-orbit interaction and the magnetic field oriented along a direction perpendicular to the plane of

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$$j_z = l_z + \frac{1}{2}\sigma_z, \quad \text{where } l_z = -i\partial_\theta \quad (41)$$

Here, the total momentum operator, $j = \pm 1/2m$ and $m = 1, 2, 3, \dots$. The eigenfunctions of the total Hamiltonian operator H in (20) can be written as^{4(a)2}

$$\psi_j(r, \theta, z) = \left[e^{i(j-1/2)\theta} g_j(r, z) \right]^{-1/2} z' \quad (42)$$

where f_j and g_j are the components of the total wave function. The total Hamiltonian H for the conduction band can be written in cylindrical coordinates by substituting the components of (42) into (20). The details of the procedure are given in Ref. [42]. So, we can write

$$H = \begin{bmatrix} h_- & \alpha_R \left[\frac{\partial}{\partial r} + \frac{1}{r} \left(j + \frac{1}{2} \right) + \frac{eB_a r}{2\hbar} \right] \\ \alpha_R \left[-\frac{\partial}{\partial r} + \frac{1}{r} \left(j - \frac{1}{2} \right) + \frac{eB_a r}{2\hbar} \right] & h_- \end{bmatrix} \quad (43)$$

$$h_- = -\frac{\hbar^2 I''}{2m_0} \left[\frac{1}{r} \frac{dr}{dj} + \frac{d}{dz} \frac{ddz}{dz} \right] + \frac{\hbar^2 I'}{2m_0 r^2} \left(j \mp \frac{1}{2} \right) + \frac{1}{2} \frac{\hbar \omega_c}{2} \left(j \mp \frac{1}{2} \right)^2 + \frac{1}{2} \frac{\hbar \omega_c}{2} \text{Mfl5n} + E(\dots) + eV + \text{all.e.} + a_f^{1/\wedge} + y + 2e^{*\wedge u_r} \quad (44)$$

The corresponding eigenvalue problem has the form

$$H|\psi_i(r, z)\rangle = e_i|A_v(r, z)\rangle \quad (45)$$

$$(h_{V^*} - \epsilon) f_j + r_R \left[\frac{d}{dr} + \frac{1}{rV} \left(j + \frac{1}{J} \right) - \frac{eB_a r}{2hJ} \right] g_j = 0 \quad (46)$$

$${}^{\text{R}}R \left| -\Lambda + \frac{1}{2} \right| \frac{eB_{\sim}}{2\hbar} \left| f_j + (h_- - \epsilon)^{\wedge=0} \right| \quad (47)$$

The diffraction of light by the periodic structure of the QDs is not directly available from reported experimental data with respect to the various parameters and geometries. These parameters include the magnetic field B_a , mechanical strain, piezoelectric potential and piezomagnetic potential at several different temperatures (see Eqs. (24)–(38) and (44)). The analytical solution of such differential equations is available only in some special simplified cases, e.g., Ref. [42].

5. RESULTS AND DISCUSSION

Electron wave functions and eigenvalues are found by solving Schrodinger Eqs. (46) and (47) with appropriate

- the influence of magneto-thermo-electromechanical effects on strain, built in piezoelectric field and potential;
- the influence of magneto-thermo-electromechanical effects on the eigenstates and spin-splitting energy.

5.1. Magneto-Thermo-Electromechanical Effects in Quantum Dots with and Without Wetting Layer

In this subsection, we focus on the study of the influence of magneto-thermo-electromechanical effects on the strain, built in piezoelectric potential and piezoelectric field in cylindrical AlN/GaN and GaN/BaTiO₃ QDs.^{20,23} For magnetic GaN/BaTiO₃ QDs, the material is doped (or assumed to be doped) with manganese (Mn) and we consider the material constants from Ref. [67] so that $f_{ij} = 0.33$ N/Am and $g_{ji} = 1$ nano-N·s/Vc. These constants are comparable to CoFe₂O₄ which indicates that Mn₃GaN is a highly wfsite (team^M^r^liteBiWlc5fh^^Ti^qaisittadiffiffi^nstants u. 07 Mar 2013 21:48:15 are not readily available from reported experimental data Scientific Publishers $f_{33} = -0.01$ N/Am, $f_{j1} = 580.3$ N/Am, $f_{33} = 699.7$ N/Am, $f_{j5} = 550$ N/Am, $g_n = 0.005$ nano-N · s/Vc and $g_{33} = 0.003$ nano-N · s/Vc.^{5,68-71} Figures 2-5 provide further insight into the influence of magneto-thermo- electromechanical effects on the strain, piezoelectric field and potentials in AlN/GaN and GaN/BaTiO₃ QDs with and without wetting layers.

In Figure 2, we first plot the r - and z -components of strain at $r = 0$ for cylindrical AlN/GaN and GaN/BaTiO₃ QDs without wetting layers at several temperatures. The results related to AlN/GaN QDs are consistent with those found in the literature (e.g., see Ref. [29] and references therein). They serve as a benchmark for the investigation of the influence of magneto-thermo-electromechanical effects on the properties of magnetic GaN/BaTiO₃ QDs. The built-in strain due to lattice mismatch in AlN/GaN QDs decreases with the increase in temperature.²⁹ However, the influence of the thermo-electromechanical effects on the magnetic GaN/BaTiO₃ QDs is not as significant as for AlN/GaN QDs. Also, the r - and z -components of strain at $r = 0$ along z -direction can be enhanced significantly in GaN/BaTiO₃ QDs (approximately for one order of magnitude) compared to the corresponding values for AlN/GaN QDs. The variation of strain due to lattice mismatch in GaN/BaTiO₃ QDs along a - and c -axes is approximately -20.1% and 28.4% respectively, whereas for AlN/GaN QDs, they are -2.4% and -3.9% . It means

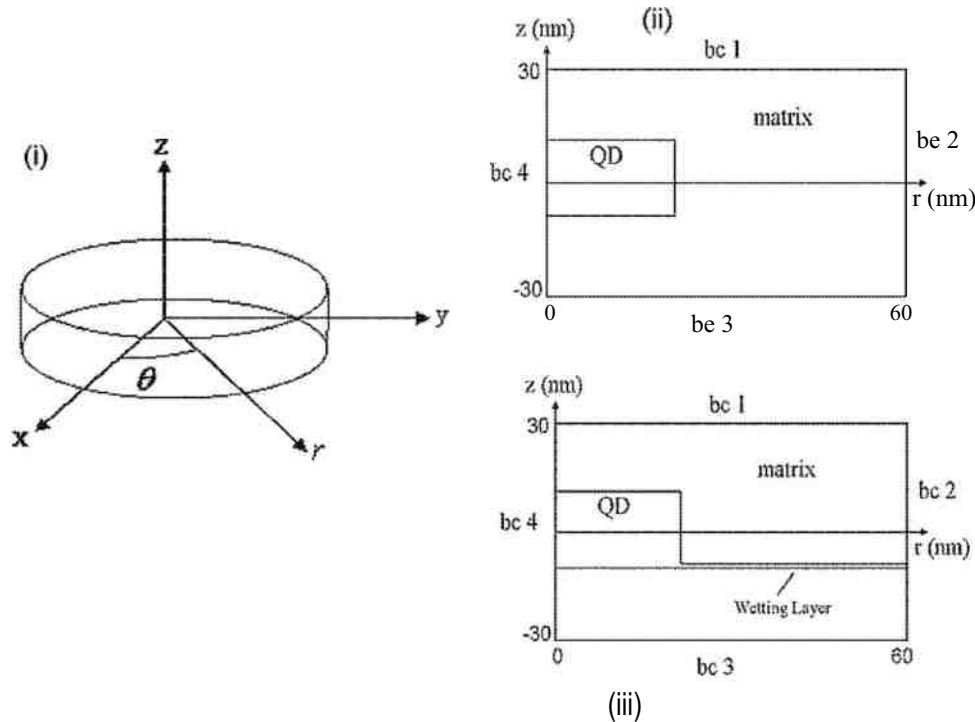


Fig. 1. The schematic diagram of the geometry of the quantum dot (see Fig. 1(i)). This two dimensional cylindrical dot with and without wetting layer is shown in Figures 1(ii) and (iii). The chosen geometry and size allow comparisons with the results available in the literature (see Refs. [29, 64]).

Table i. EMItMeitdn^nRidbl^iag Technology to Hniuensite de Montreal - fibNrofiScpes - Acquisition (PER) the same as in Ref. [291, The material coHSanl^ J204)^ 84oW6tQn: ThQfOTWfr^e 13-2^485^ along «^axis and 24.5% higher are taken from Refs. [5,68-71]. Copyright American SGlengh&iRilblshffirts gives the enhancement with the variation of strain in magnetic QDs.

Material constants	AlN	GaN	BaTiO ₃
Stiffness			
coefficients (GPa)			
*11	396	390	166 [68]
*12	137	145	77 [68]
*15	108	106	78 [68]
*c11	373	398	162 [68]
*44	116	105	43 [68]
Permittivity			
*11	8.67	9.28	1265 [68]
*c11	8.57	10.02	1423 [68]
Piezoelectric			
coefficients (Cm ⁻²)			
*15	-0.6	-0.49	11.6 [68]
*51	-0.6	-0.49	-4.4 [68]
*55	1.46	0.73	18.6 [68]
Pyroelectric			
coefficients (Cm ⁻² K ⁻¹)			
r _s x 10 ⁻⁶	7.5	0.91	-19.72 [5]
Thermal stress			
constants (PaK ⁻¹)			
A _n x 10 ⁵	-4.44	5.57	6.21 [69]
A _{s,s} x 1(F	6.9	-8.66	5.51 [69]
Lattice constant (Å)			
a	3.112	3.189	3.992 [70,71]
c	4.982	5.185	4.036 [70,71]
Spontaneous	-0.081	-0.029	-0.26 [20]
polarization (Cm ⁻²)			

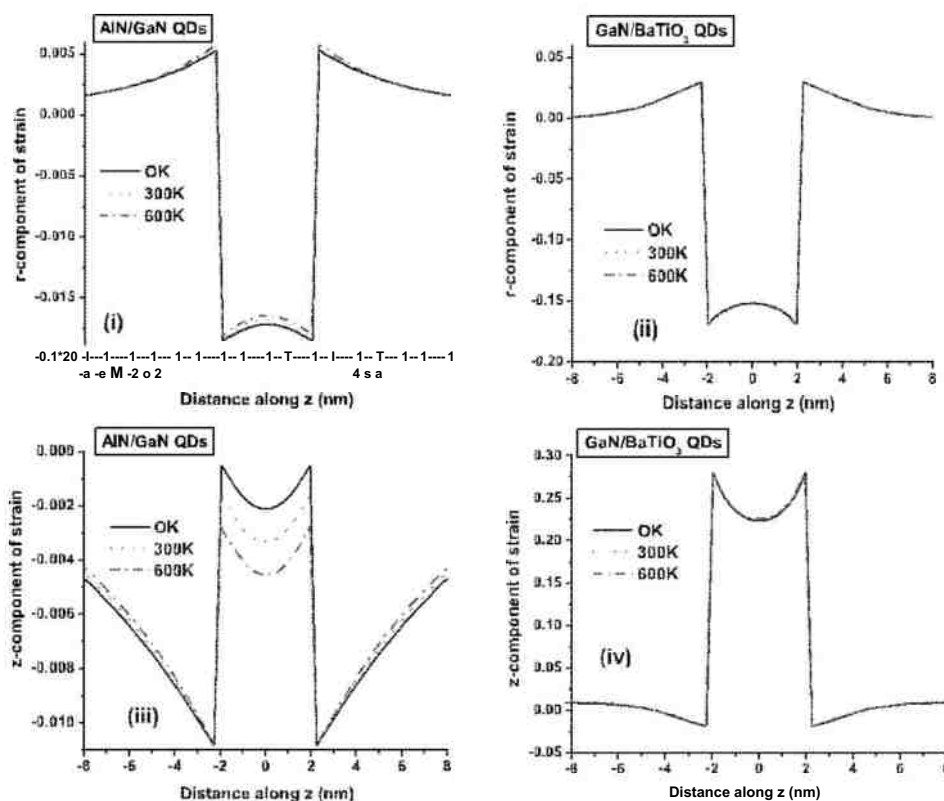


Fig. 2. The influence of thermo-electromechanical effects on the properties of cylindrical AlN/GaN and GaN/BaTiO₃ QDs. Upper panel represents the r -component of strain versus distance along z -direction at $r = 0$ and lower panel represents the z -component of strain versus distance along z -direction at $r = 0$. It can be seen that this component of strain in the magnetic BaTiO₃ QDs is independent of temperature. Here we choose $B_a = 0$.

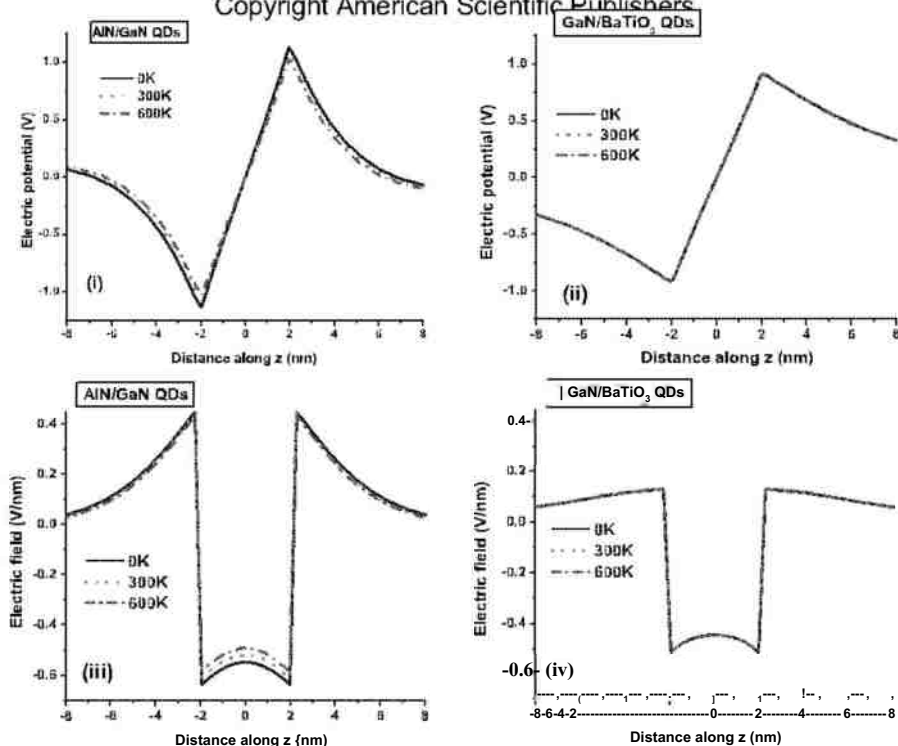


Fig. 3. The influence of thermo-electromechanical effects on the properties of cylindrical AlN/GaN and GaN/BaTiO₃ QDs. Upper panel represents the electric potential versus distance along z -direction at $r = 0$ and lower panel represents the electric field versus distance along z -direction at $r = 0$. Again, it can be seen that the electric field in the magnetic BaTiO₃ QDs is independent of temperature. Here we choose $B_a = 0$.

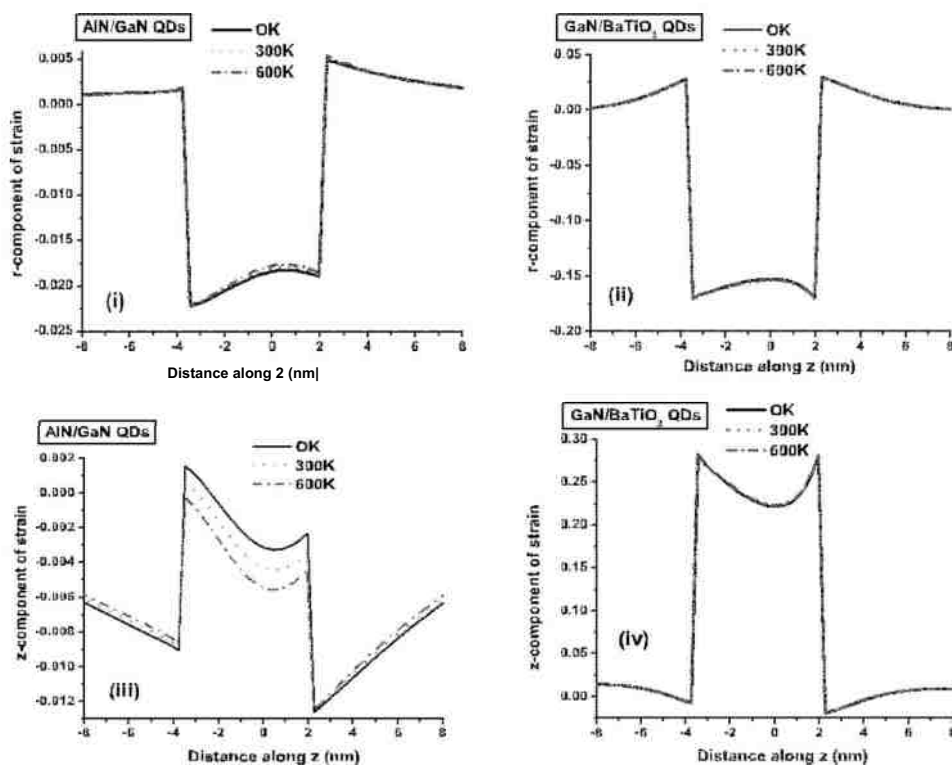


Fig. 4. The influence of wetting layers on the properties of cylindrical AlN/GaN and GaN/BaTiO₃ QDs. Upper panel represents the r -component of strain versus distance along z -direction at $r = 0$ and lower panel represents the z -component of strain versus distance along s -direction at $r = 0$. It can be seen that the influence of wetting layers on the strain part has almost no effect for the magnetic BaTiO₃ QDs. Here we choose $B_z = 0$.

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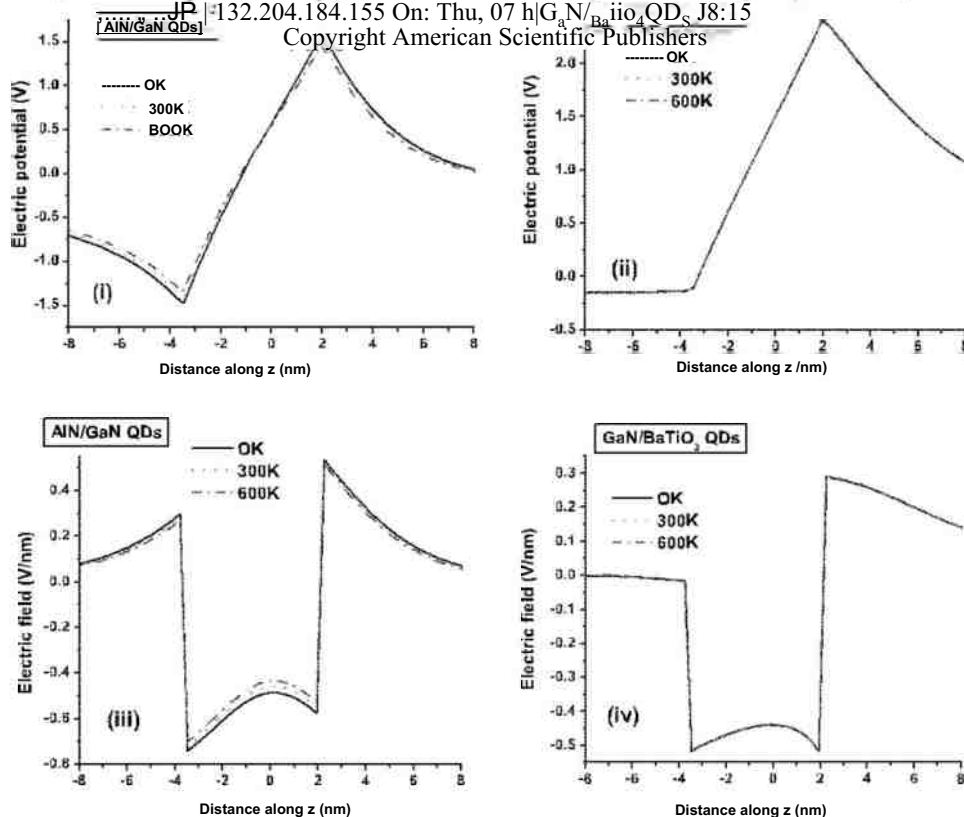


Fig. 5. The influence of wetting layers on the properties of cylindrical AlN/GaN and GaN/BaTiO₃ QDs. Upper panel represents the electric potential versus distance along z -direction at $r = 0$ and lower panel represents the electric field versus distance along z -direction at $r = 0$. Here we choose $B_z = 0$.

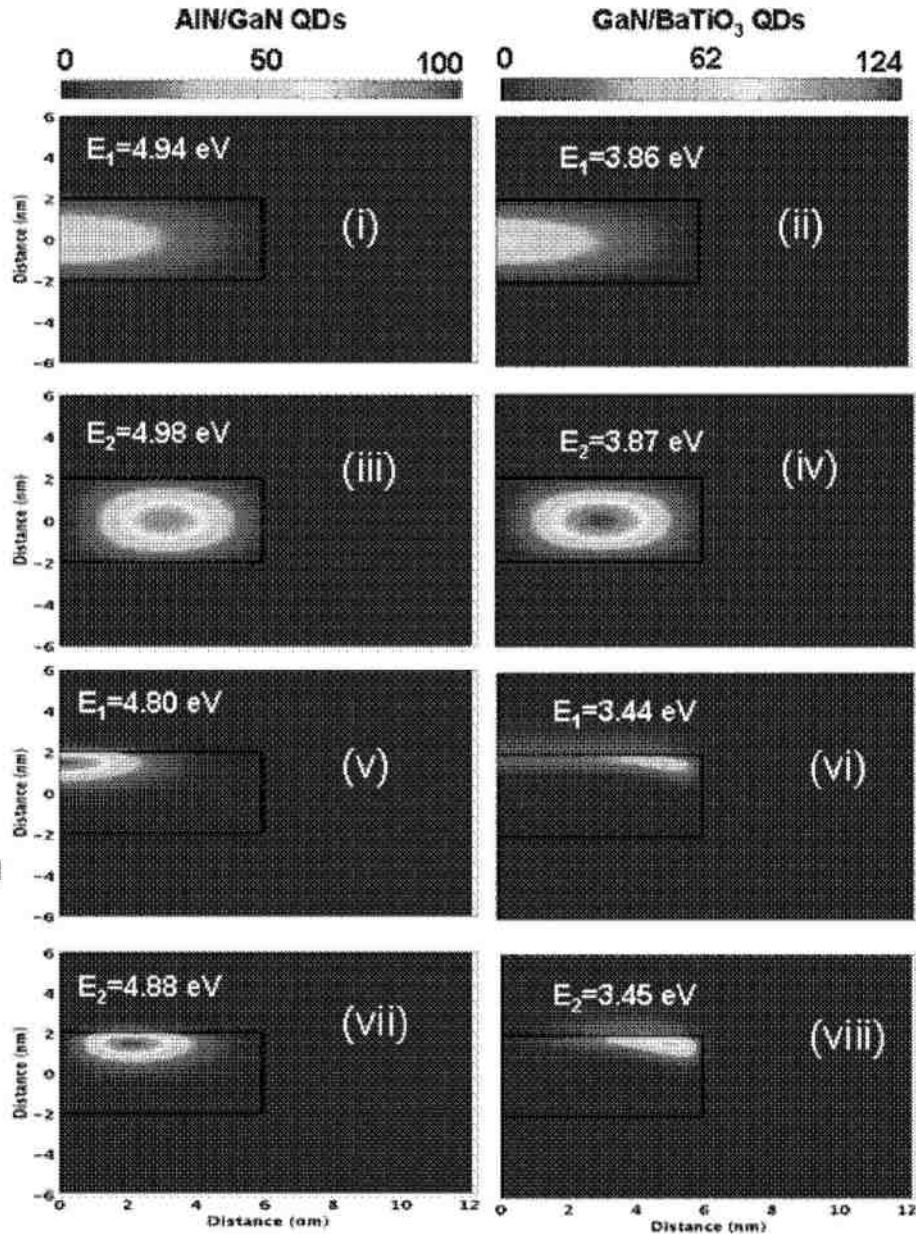


Fig- 6. The influence of electromechanical effects on the band structures of cylindrical AlN/GaN and GaN/BaTiO₃ QDs. Figures 5(i)-(iv) represent the ground and first excited state wave functions without the inclusion of electromechanical effects and Figures 6(v)-(vi) represent these functions with the inclusion of electromechanical effects. It can be seen that piezoelectromechanical effects bring the electron wave functions to the top of the dot. Electron wavefunctions in magnetic QDs are quite different compared to AlN/GaN QDs (see Figs. 6(v)-(viii)). Further explanations are given in the text. Here we choose $T = 0$ and $B_z = 0$.

5.2. Magnetoelectric and Piezomagnetic Quantum Dots

Next, we will highlight the results of our study on the influence of magneto-thermo-electromechanical effects in the band structure calculations of cylindrical AlN/GaN and GaN/BaTiO₃ QDs. The idea is to dope the materials with Mn to enhance the magnetoelectric and piezomagnetic properties of GaN/BaTiO₃ QDs.⁶⁷ We have also suggested to dope the GaN materials with Al so that the band gap becomes slightly larger than for BaTiO₃ materials. As it

was pointed out before,⁴³ BaTiO₃ material can be treated in such cases as a QD.

We apply a multi-physics simulation strategy based on the finite element method⁴⁴ to provide a realistic description of the band diagram of AlN/GaN QDs. The idea is to first solve the coupled system equations of (24) through (28) in cylindrical coordinates for magnetic QDs to get the realistic electromechanical strain, piezoelectric and piezomagnetic potentials. After that, we implement the electromechanical effects in the band structure calculations of cylindrical QDs with and without wetting layers.

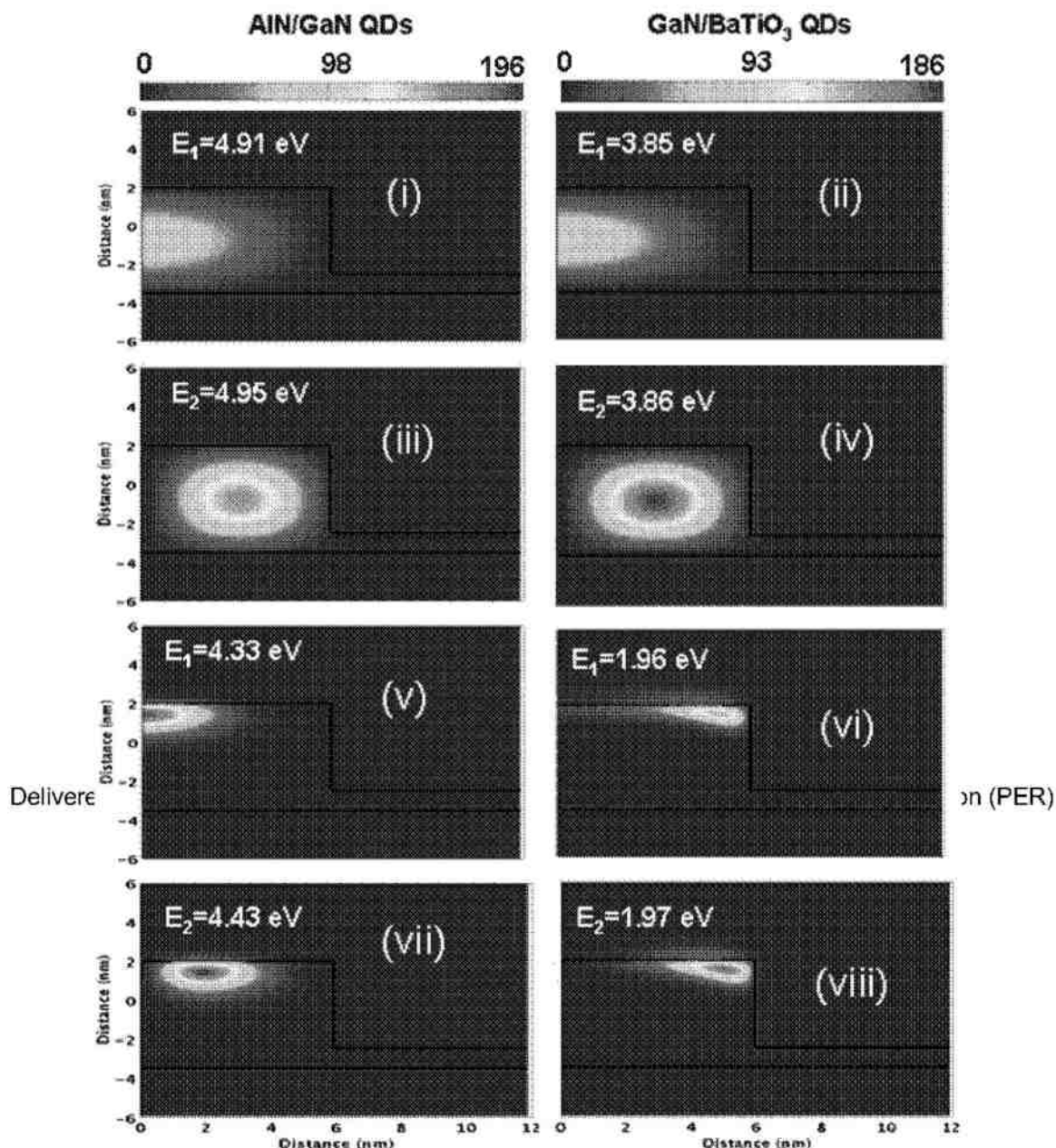


Fig. 7. The influence of electromechanical effects on the band structures of cylindrical AlN/GaN and GaN/BaTiO₃ QDs with wetting layers. Figures 7(i)-(iv) represent the ground and first excited state wave functions without the inclusion of electromechanical effects and Figures 6(v)-(vi) represent these functions with the inclusion of electromechanical effects. It can be seen that piezoelectromechanical effects bring the electron wave-functions to the top of the dot. Eigenvalues are found noticeably lower in magnetic QDs in the case with wetting layers (Figs. 7(vi) and (viii)) than for the case without wetting layers (Figs. 6(vi) and (viii)). Further explanations are given in the text. Here we choose $T = 0$ and $B_a = 0$.

The numerical parameters for AlN/GaN and GaN/BaTiO₃ QDs are taken from Refs. [29 and 43], respectively (see also references therein).

5.2.1. Influence of Magneto-Thermo-Electromechanical Effects on the Eigenstates

We add piezoelectric potential (Figs. 3(i), (ii) and 5(i), (ii)) to the flat band diagram of AlN/GaN and GaN/BaTiO₃ QDs and consider the combined influence

of magneto-thermo-electromechanical effects as a tuning parameter in modifying the band diagram. We solve the coupled Schrödinger Eqs. (46) and (47) to get the wave functions and the eigenvalues of the QDs.

The in plane wave functions of the QDs without WLs in the flat band diagram are shown in Figures 6(i)-(iv). It can be seen that the wave functions are localized at the center of the QDs, indicating that the magneto-electromechanical effects are not accounted for in the band diagram. The influence of magneto-electromechanical effects on the

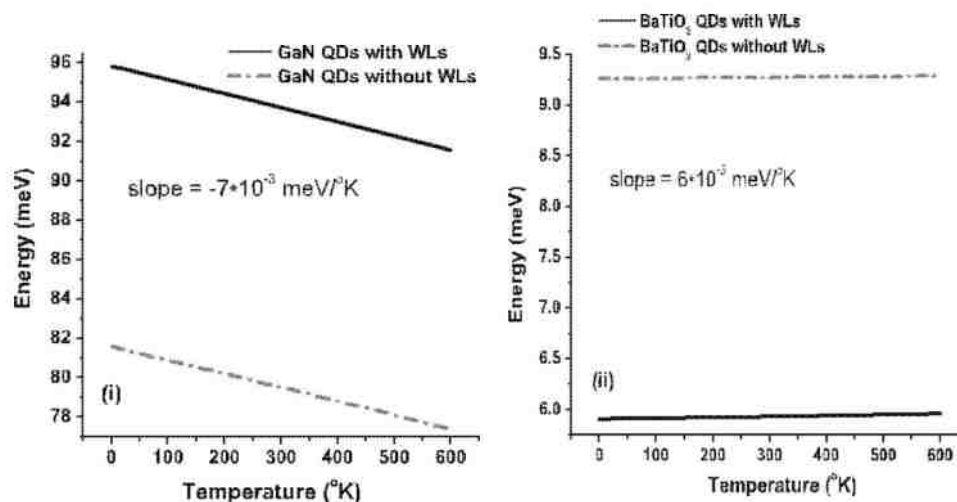


Fig. 8. Intra-subband energy difference versus temperature in GaN and BaTiO₃ QDs with and without wetting layers. It can be seen that in the magnetic BaTiO₃ QDs, the energy difference as a function of temperature is approximately two order of magnitude smaller compared to its values for GaN QDs.

wave functions and on the eigenstates are shown in Figures 6(v)-(viii). It can be seen that the influence of magneto-electromechanical effects pushed the localized wave functions to the top of the QDs. The influence of the magneto-electromechanical effects on the wave functions

of the magnetic BaTiO₃ QDs is quite different (Figs. 6(vi), (viii)) than for GaN QDs (Figs. 6(v), (vii)). This confirms the proposal for using the magneto-electromechanical effects as a tuning parameter in controlling the localized wave functions and eigenvalues in the magnetic QDs.

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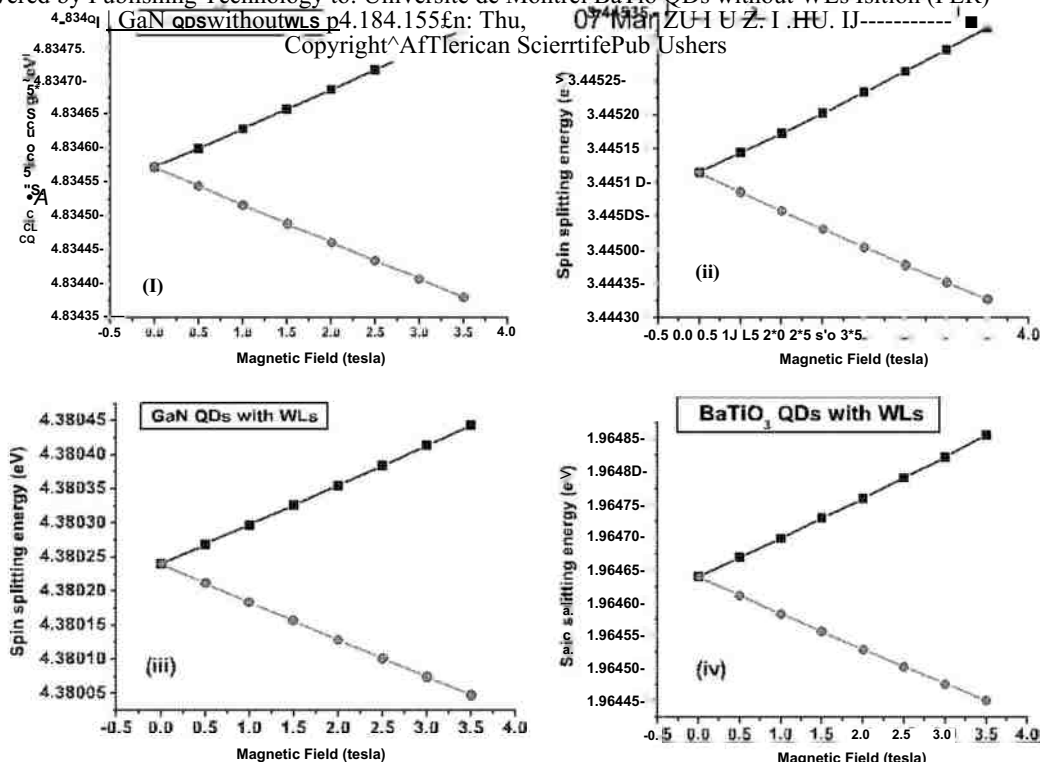


Fig. 9. The spin splitting energy between two lowest eigenstates versus magnetic field at room temperature ($T = 300$ K) in AlN/GaN and GaN/BaTiO₃ QDs for two different cases: without WLs (Figs. 9(i), (ii)) and with WLs (Figs. 9(iii), (iv)). In Figure 9, we plotted the ground state energy of spin down electron for the quantum number $j = 1/2$ (shown by solid lines with diamond) and ground state energy of spin up electron for the quantum number $j = -1/2$ (shown by solid lines with circle). Here we consider $a_K = 5 \times 10^{-4}$ eV nm as the Rashba coefficient value.

The influence of wetting layers on the eigenvalues and wave functions of the QDs are shown in Figure 7. Similar to Figure 6, the in plane wave functions of the QDs with WLs in the flat band diagram are shown in Figures 7(i)-(iv) and the influence of magneto-electromechanical effects is demonstrated in Figures 7(v)-(viii). It can be seen that the eigenvalues for the magnetic QDs with WLs are noticeably smaller (see Figs. 7(vi), (viii)) than for the case without WLs (see Figs. 6(vi), (viii)). The reason behind smaller eigenvalues in magnetic QDs with WLs is that the magneto-electromechanical effects push the flat band diagram down (Figs. 5 (ii), (iv)) in a more pronounced way than in the case without WLs (Figs. 3(ii), (iv)).

Figure 8 provides further information on the intra-subband energy (i.e., the energy difference between the ground and first excited states) versus temperature for both AlN/GaN and GaN/BaTiO₃ QDs with and without wetting layers. It is clear that the variation in the slope is two order of magnitude smaller in the magnetic GaN/BaTiO₃ QDs than in AlN/GaN QDs which indicates that the magnetic QDs are less sensitive to temperature.

5.2.2. The Spin Splitting Energy in QDs with and without Wetting Layers

We now turn to a presentation of another important result of this work: the spin splitting energy of ground and first excited states. Figure 9 shows the spin splitting energy of ground and first excited states versus magnetic field for AlN/GaN and GaN/BaTiO₃ QDs with and without wetting layers.

In the absence of the magnetic field, as it is clear from (43), there is an additional asymmetry at $j_z \rightarrow -j_z$ due to the time inversion. It means that the eigenstates with the projection of total angular momentum equal to j and $-j$ are Kramer's degenerate. In Figures 9(i), (ii), we find the ground state Kramer's degenerate eigenvalues at 4.83 eV for AlN/GaN QDs and 3.44 eV for GaN/BaTiO₃ QDs without wetting layers. These results have been obtained by directly solving the coupled Schrödinger Eqs. (46) and (47). Here we consider $j = 1/2$ in Eq. (46) and $-j = -1/2$ in Eq. (47). In the presence of magnetic field along z -direction, there is no degeneracy and we obtain the spin splitting energy. In the presence of wetting layers in the QDs (Figs. 9(iii), (iv)), Kramer's degenerate eigenvalues and spin splitting energy occur at lower values. We found that the divergence in the Zeeman spin splitting energy increases with the increase in magnetic field due to the Rashba spin-orbit coupling in both cases: QDs with wetting layers and without wetting layers.

Finally, in Figure 10, we plotted the spin splitting energy difference of the ground and first excited states versus magnetic field in the QDs. Here we solved the Schrödinger Eqs. (46) and (47) to get the ground state eigenvalues for $j = 1/2$ and $j = -1/2$. We keep the Rashba coefficient value at $a_R = 5 \times 10^{-4}$ eV nm. There is a slight variation in the spin splitting energy difference versus magnetic field

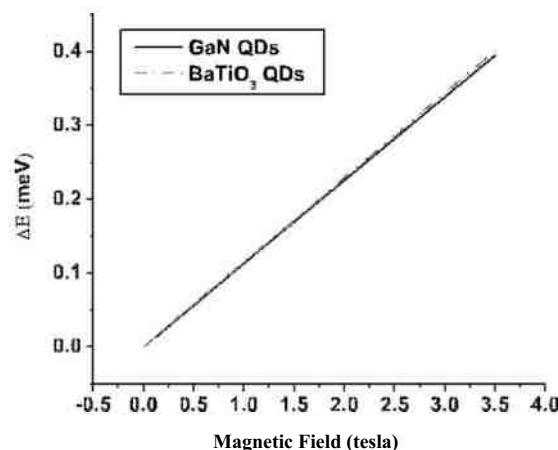


Fig. 10. The spin splitting energy difference versus magnetic field of AlN/GaN (solid line) and GaN/BaTiO₃ (dashed-dotted line) QDs at room temperature (i.e., at $T = 300$ K).

in magnetic BaTiO₃ compared to GaN QDs. The spin splitting energy difference is controlled by the Zeeman term ($g_0 \mu_B B$, see Eq. (21)) and it is increased with the increase in the magnetic field. However, the variation in the spin splitting energy difference between GaN and BaTiO₃ QDs is mainly due to the variation in the bulk value of g -factor. Note that the bulk g -factor for GaN material is 1.9566 and for BaTiO₃, we consider free electron

g -factor, i.e. 2.

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6. CONCLUSIONS

We have carried out a systematic study of the influence of the magneto-thermo-electromechanical effects on the properties of QDs with and without WLs. In this study, we have covered three different groups of nanostructures such as ferroelectric, piezomagnetic and piezoelectric QDs.

Firstly, we have analyzed in detail the influence of magneto-thermo-electromechanical effects on the strain, electric field and electric potential of cylindrical AlN/GaN and GaN/BaTiO₃ QDs with and without wetting layers. We have shown (see Figs. 2, 4) that the ϵ_z -components of strain at $r = 0$ along z -direction can be enhanced significantly due to higher lattice mismatch along z -direction for ferroelectric QDs compared to piezoelectric QDs. Also, piezoelectric and stiffness coefficients of ferroelectric QDs are much smaller than their counterparts in piezoelectric QDs. This causes a decrease in electric potential and electric field for ferroelectric QDs in comparison to piezoelectric QDs (see Figs. 3, 5).

Secondly, we have analyzed the influence of magneto-thermo-electromechanical effects on the band structures of cylindrical AlN/GaN and GaN/BaTiO₃ QDs with and without wetting layers (see Figs. 6-8). While it has been demonstrated that the wetting layer has a significant effect on the modification of strain, electric field and electric potential, we have also demonstrated that it modifies the

band diagram and localized eigenstates of the QDs. Furthermore, we have accounted for the magneto-thermoelectric effect in the band structure of magnetic QDs in the presence of spin-orbit interaction and employed a fully coupled numerical approach to obtain the eigenvalues and eigenstates based on the finite element method.

Finally, as demonstrated by Figures 9 and 10, we have carried out a numerical simulation study of the spin split energy in magnetic AlN/GaN and GaN/BaTiO₃ QDs with and without WLs. We have shown that in the presence of externally applied magnetic field along z-direction, the spin splitting energy in magnetic QDs with WLs can be shifted significantly to the lower energy levels in magnetic QDs with WLs.

Acknowledgments: This work was supported by the Ikerbasque, Spain, the University of Jyväskylä, Finland and by the NSERC and CRC program, Canada.

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Received: 27 December 2011. Accepted: 29 January 2012.