Electromechanical fields in GaN/AlN Wurtzite Quantum Dots

D. Barettin, B. Lassen, and M. Willatzen
Mads Clausen Institute for Product Innovation, University of Southern Denmark
Alsion 2, Dk - 6400 Sønderborg, Denmark

Abstract. We show that the governing equations for the electromechanical fields of wurtzite structures are axisymmetric, hence all electric- and mechanical-field solutions are axisymmetric as well and the original three-dimensional problem can be solved as a two-dimensional mathematical-model problem \[1\]. We present results of the combined influence of lattice mismatch, piezoelectric effects, and spontaneous polarization for wurtzite (WZ) structures consisting of a GaN quantum dot embedded in a AlN matrix.

1. Introduction
GaN/AlN quantum dot (QD) structures have recently received much attention due to their relevance for optoelectronic devices \[3\]. An important aspect in this context is the influence of electromechanical-field interactions and their combined effects on the bandstructure and eigenstates of QDs. In this paper, we develop a two-dimensional mathematical model for computing the electromechanical fields of a GaN/AlN QD showing the importance of piezoelectric effects, spontaneous polarization, and lattice mismatch with quantitative comparisons. Also we present a comparison with one-dimensional analytical results for coupled and uncoupled fields. The paper is organized as follow. In section 2, we write the governing and equilibrium equations in cylindrical coordinates due to the system’s rotational invariance. In section 3, we present numerical results for the electromechanical fields and a quantitative comparison is carried out. A comparison with one-dimensional analytical results is also highlighted.

2. Governing equations and analytical results for electromechanical fields
The stress tensor in a crystal is given by (with \(\partial_n\) being the derivative along direction \(n\)):

\[
\sigma_{ik} = C_{iklm} \varepsilon_{lm} + e_{nik} \partial_n V, \tag{1}
\]

while the electrical displacement is:

\[
D_i = e_{ilm} \varepsilon_{lm} - \hat{\varepsilon}_{in} \partial_n V + P_{sp}, \tag{2}
\]

where \(C_{iklm}, e_{nik}, \hat{\varepsilon}_{in}, \varepsilon_{lm}, V, P_{sp}\) are the constants of elastic moduli, the piezoelectric constants, the permittivities, the strain tensors, the electrical potential and the spontaneous polarization respectively \[4\]. The linearly independent elastic constants and piezoelectric constants in a crystal with WZ symmetry are \[2\]:

\[
\begin{align*}
C_{1111} &\equiv C_{11}; & C_{1122} &\equiv C_{12}; & C_{1133} &\equiv C_{13}; \\
C_{3333} &\equiv C_{33}; & C_{2323} &\equiv C_{44}; & C_{2121} &\equiv (C_{11} - C_{12})/2; \\
e_{3111} &\equiv e_{31}; & e_{3333} &\equiv e_{33}; & e_{1133} &\equiv e_{15}. \tag{3}
\end{align*}
\]
To take into account lattice mismatch, the strain tensor is represented as [2]:

$$\varepsilon_{ij} = \varepsilon_{ij}^{(u)} + \varepsilon_{ij}^{(0)},$$ (4)

where $\varepsilon_{ij}^{(0)}$ is the tensor of local intrinsic strain (lattice mismatch) and $\varepsilon_{ij}^{(u)}$ is the local strain tensor dependent on positions given by:

$$\varepsilon_{ij}^{(0)} = (\delta_{ij} - \delta_{iz}\delta_{jz})a + \delta_{iz}\delta_{jz}c$$ $\varepsilon_{ij}^{(u)} = \frac{1}{2}(\partial_j u_i + \partial_i u_j),$$ (5)

with $a = \frac{a_m-a_{QD}}{a_m}$ and $c = \frac{c_m-c_{QD}}{c_m}$ in the dot and zero otherwise. Here $a_m$, $c_m$, and $a_{QD}$, $c_{QD}$ are the lattice constants of the matrix and the QD, respectively [2].

In cylindrical coordinates the constitutive relations take the form:

$$\begin{align*}
\sigma_{rr} &= C_{11}\varepsilon_{rr} + C_{12}\varepsilon_{\varphi\varphi} + C_{13}\varepsilon_{zz} + (C_{11} + C_{12})a + C_{33}c + e_{31}\partial_z V, \\
\sigma_{\varphi\varphi} &= C_{11}\varepsilon_{\varphi\varphi} + C_{12}\varepsilon_{rr} + C_{13}\varepsilon_{zz} + (C_{11} + C_{12})a + C_{33}c + e_{31}\partial_z V, \\
\sigma_{zz} &= C_{33}\varepsilon_{zz} + C_{13}(\varepsilon_{rr} + \varepsilon_{\varphi\varphi}) + 2C_{13}a + C_{33}c + e_{33}\partial_z V, \\
\sigma_{r\varphi} &= (C_{11} - C_{12})\varepsilon_{r\varphi}, \\
\sigma_{\varphi z} &= 2C_{44}\varepsilon_{\varphi z} + e_{15}(1/r)\partial_r V, \\
\sigma_{rz} &= 2C_{44}\varepsilon_{rz} + e_{15}\partial_r V, \\
D_r &= 2e_{15}\varepsilon_{rz} - \varepsilon_{11}\partial_r V, \\
D_\varphi &= 2e_{15}\varepsilon_{\varphi z} - \varepsilon_{11}(1/r)\partial_r V, \\
D_z &= e_{31}(\varepsilon_{rr} + \varepsilon_{\varphi\varphi}) + e_{33}\varepsilon_{zz} - \varepsilon_{33}\partial_z V + P_{sp},
\end{align*}$$ (6)

The static Navier’s equations read:

$$\partial_j \sigma_{ij} = 0.$$ (7)

In the absence of external charges, the electrical potential is found by solving the Maxwell equation [2]:

$$\partial_i D_i = 0.$$ (8)

From (7) and (8) we obtain a set of coupled equilibrium equations for the strain and the electrical fields in cylindrical coordinates:

$$\begin{align*}
\partial_r \sigma_{rr} + (1/r)\partial_\varphi \sigma_{\varphi\varphi} + \partial_\varphi \sigma_{\varphi z} + (1/r)(\sigma_{rr} - \sigma_{\varphi\varphi}) &= 0, \\
\partial_r \sigma_{r\varphi} + (1/r)\partial_\varphi \sigma_{\varphi\varphi} + \partial_\varphi \sigma_{\varphi z} + (2/r)\sigma_{r\varphi} &= 0, \\
\partial_r \sigma_{rz} + (1/r)\partial_\varphi \sigma_{\varphi z} + \partial_\varphi \sigma_{zz} + (1/r)\sigma_{rz} &= 0, \\
\partial_r D_r + (1/r)D_\varphi + \partial_\varphi D_z &= 0.
\end{align*}$$ (9)

These equations are invariant with respect to rotations around the z axis (in spite of the lack of axisymmetry of the underlying wurtzite lattice, refer to detailed discussions in Ref. [5]), hence solutions can be separated into a $(r, z)$ part and a $\varphi$ part.

In Figure 1 we plot the three-dimensional geometry of the QD under consideration (left) and the $(r, z)$ representation (right). Dirichlet boundary conditions are imposed along bc: 1, 2, and 3 while $u_r = 0$, $\partial_r u_z = 0$ and $\partial_z V = 0$ at bc 4.

Due to the axisymmetry of the system (equations, geometry and boundary conditions) there is no angular dependence and $u_\varphi = 0$. We write the remaining equations in following instructive form:

$$L\psi = f,$$ (10)
Figure 1. Geometry of the system considered (left) and of the two-dimensional model (right)

where \( \psi \equiv (u_r, u_z, V) \), \( L \) is the second-order differential operator given in the appendix, and \( f \) is the source term given by

\[
\begin{bmatrix}
-\partial_r [(C_{11} + C_{12}) a + C_{33} c] \\
-\partial_z [2C_{13} a + 2C_{13} c] \\
-\partial_z P_{sp}
\end{bmatrix}.
\]

(11)

Because the functions appearing in the source term are piecewise constant what we in reality have are surface sources for the strain and the electric potential (the discontinuities appear at the interfaces).

3. Numerical results

We present results for a cylindrical GaN QD with a radius of 6 nm and an height of 3 nm embedded in a matrix with a radius of 60 nm and an height of 30 nm of AlN. It has been checked that the boundary is so far away from the dot that it does not influence the field distributions significantly. Results for the four following cases will be compared in this section:

- Case 1: With lattice mismatch, piezoelectric effect, and spontaneous polarization.
- Case 2: With lattice mismatch and piezoelectric effect.
- Case 3: With piezoelectric effect and spontaneous polarization.
- Case 4: Lattice mismatch only.

In Figure 2, we plot \( u_r(r) \) for \( z = 0 \) (left) and \( u_z(z) \) for \( r = 0 \) (right). By comparing cases 1, 2, and 4, it is seen that lattice mismatch is the main driving force for the strain-distribution while piezoelectricity and spontaneous polarization are of less importance. This is also clear from the source term (Equation (11)). This was also shown in [6] but for the 1D case of a GaN quantum well surrounded by AlN layers. However, for an AlN quantum well surrounded by GaN, piezoelectric and spontaneous polarization contributions to strain are important (more than 30% in absolute values of the lattice mismatch contribution, refer to [6]). The present 3D analysis confirms that contributions from piezoelectric and spontaneous polarization amount to approximately 30% of the lattice mismatch. However, since spontaneous polarization and piezoelectricity destroy inversion symmetry, the solutions to the set of partial-differential equations in general do not satisfy parity. This is indeed found in cases 1-3 as the electric field (displacement vector) is even (odd) with respect to inversion (see also the figures 4 and 5). In the inversion symmetry case (case 4), the electric field is zero and the displacement vector is odd with respect to inversion.
Figure 2. Displacement vectors $u_r(r)$ for $z = 0$ (left) and $u_z(z)$ for $r = 0$ (right).

In Figure 3 we plot the strain tensors $\varepsilon_{rr}$ and $\varepsilon_{zz}$ at $r = 0$ and at $z = 0$ for the various cases and in Figure 4 we show two-dimensional plots of the strains $\varepsilon_{rr}$ (left), $\varepsilon_{zz}$ (center), and $\varepsilon_{rz}$ (right). From these figures we see that the dot material is compressed by the barrier material and the barrier material close to the dot is compressed by the dot material. This is in accordance with what is observed in other systems and it can be understood from the conceptual idea of preparing the system with a shrink fit procedure [9].

It should also be mentioned that the $\varepsilon_{rz}$ component is divergent at the corners, however, the solution away from the corners are still expected to be reasonable [10]. From Figure 3 it is clear that the most pronounced difference between case 1 and the cases 2 and 4 is to be found along the $z$-direction. This difference is due to spontaneous polarization and as the spontaneous polarization is directed along the $z$-axis this is expected.

It is interesting to make a comparison between our results for the three-dimensional system and analytical results for the simpler one-dimensional case [6]. We compare results not only for the previous system: A GaN QD embedded in a matrix of AlN (GaN/AlN), but also for an AlN QD embedded in a matrix of GaN (AlN/GaN) [11].

The analytical expression for the stress tensor in one dimension can be written as a sum of three terms: (1) an uncoupled term due to mechanical fields only, (2) a coupled piezoelectric term combining electrical and mechanical fields, and (3) a term due to couplings between spontaneous polarization and piezoelectricity. If we identify the QD as layer (1) and the matrix as layer (2) we can write [6]:

$$
\varepsilon_{zz}^{(1)} = \frac{2C_{13}^{(1)}}{C_{33}^{(1)}} - \varepsilon_{33}^{(1)} + \frac{C_{13}^{(1)} e_{33}^{(1)} - e_{33}^{(1)} C_{33}^{(1)}}{C_{33}^{(1)} e_{33}^{(1)} + (e_{33}^{(1)})^2} a + \frac{C_{13}^{(1)} (P_{sp}^{(2)} - P_{sp}^{(1)})}{C_{33}^{(1)} (e_{33}^{(1)} + (e_{33}^{(1)})^2)},
$$

(12)

$$
\varepsilon_{zz} = \varepsilon_{zz}^{uncoupled} + \varepsilon_{zz}^{coupled} + \varepsilon_{zz}^{sp}.
$$

(13)

In an analogous way, one finds for the $z$ component of the electric field for the coupled and the uncoupled cases [7] (setting $e_{ij} = 0$):

$$
E_{z}^{uncoupled,1} = \frac{P_{sp}^{(2)} - P_{sp}^{(1)}}{\varepsilon_{33}^{(1)}},
$$

(14)
Figure 3. Strain tensors $\varepsilon_{rr}$ (top left) and $\varepsilon_{zz}$ (top right), at $r = 0$ and $\varepsilon_{rr}$ (bottom left) and $\varepsilon_{zz}$ (bottom right) at $z = 0$.

$$E_{z}^{\text{coupled,1}} = \frac{2[\varepsilon_{33}^{(1)} C_{13}^{(1)} - \varepsilon_{13}^{(1)} C_{33}^{(1)}]}{\varepsilon_{33}^{(1)} C_{33}^{(1)} + (\varepsilon_{13}^{(1)})^2}a + C_{33}^{(1)} \frac{P_{sp}^{(1)}}{\varepsilon_{33}^{(1)} (e_{33}^{(1)})^2}.$$  (15)

In Table 1, we present results for the strain tensor for the 1D case and the present 3D model corresponding to $r = 0$ and $z = 0$ introducing:

$$\Delta \varepsilon = \frac{\varepsilon_{zz}(3D) - \varepsilon_{zz}(1D)}{\varepsilon_{zz}(1D)}.$$  (16)

and in Table 2 we list the electric field for the uncoupled and the coupled cases (1D) and the 3D result (evaluated at $r = 0$ and $z = 0$) in addition to the relative difference $\Delta E$ defined in a similar manner as $\Delta \varepsilon$. The data for strain in [6] are for a AlN/GaN quantum-well structure while the present structure is a GaN/AlN quantum-dot structure. Hence, results cannot be expected to be quantitatively similar but they do provide a qualitative comparison between the 1D and 3D strain cases. It should be mentioned that the 1D strain results (refer to Eq.(19) in [6]) are independent of the quantum-well thickness. Results for the
Figure 4. Strains $\varepsilon_{rr}$ (top left), $\varepsilon_{zz}$ (top right), and $\varepsilon_{rz}$ (bottom) in the $r$, $z$ plane. All the effects have been included.

Figure 5. The $z$ (left) and $r$ (right) components of the electric field in the $r$, $z$ plane.

strain (Table 1 in the present work) are also given in Table 1 of [6] while electric field values (Table 2 in the present work) were calculated but not listed in [6]. Here, we would also like to correct a wrong sign in [6] for the coupled strain value of GaN/AlN (+0.008). The correct sign should read (-0.008) as given in this work.
Table 1.  $\varepsilon_{zz}$ strain values in the different (one-dimensional) cases considered, the total 1D value, the corresponding 3D value at $r=0$ and $z=0$ (3D), and the difference in percentage between a 1D and a 3D analysis ($|\Delta_\varepsilon|$).

| System      | $\varepsilon_{zz}^{\text{uncoupled}}$ | $\varepsilon_{zz}^{\text{coupled}}$ | $\varepsilon_{zz}^{\text{sp}}$ | $\varepsilon_{zz}(1D)$ | $\varepsilon_{zz}(3D)$ | $|\Delta_\varepsilon|$ |
|-------------|--------------------------------------|--------------------------------------|---------------------------------|------------------------|------------------------|-------------------|
| GaN/AlN     | 0.0123                                | -0.0008                              | -0.0014                         | 0.0101                 | -0.0050                | 150%              |
| AlN/GaN     | -0.0143                               | 0.0026                               | 0.0026                          | -0.0091               | 0.0068                | 175%              |

Table 2. Electric-field z-component for the uncoupled and coupled cases (1D) compared to the present 2D results evaluated at $r=0$ and $z=0$.

| System      | $E_z^{\text{uncoupled}}$ (GV/m) | $E_z^{\text{coupled}}$ (GV/m) | $E_z(3D)$ (GV/m) | $|\Delta E|$ |
|-------------|---------------------------------|-----------------------------|-----------------|-----------|
| GaN/AlN     | -0.608                          | -0.980                      | -0.613          | 37%       |
| AlN/GaN     | 0.716                           | 1.309                       | 0.765           | 42%       |

Note the big relative impact of employing a 3D analysis as compared to a 1D analysis on both strains and electric-field values ($|\Delta_\varepsilon|$ is numerically larger than 100%). Note also that for the AlN/GaN system, important contributions to the strain result from the piezoelectric and spontaneous-polarization coupling effects. It is instructive to observe that the latter two coupling contributions compensate, albeit slightly, for the big difference between the 1D and 3D results.

Further note that the strain is compressive in the 3D case whereas in the 1D case it is tensile for the GaN/AlN system. In the 1D case the expansion in the $z$-direction is due to the Poisson effect (the substrate compresses the material perpendicular to the $z$ axis resulting in an expansion in $z$-direction) [8]. In the 3D case the dot is not free to expand in the $z$-direction due to the presence of matrix material at the sides of the dot (and the opposite applies to the AlN/GaN system). This is the main reason behind the pronounced difference observed. From Table 2 we see that the electric field in the 1D and the 3D case has the same direction but the magnitude is smaller in the 3D case. The reason for this is twofold. First, we saw in Table 1 that there is a substantial difference in the strain between the 1D and the 3D cases. This will also change the electric field due to the coupling in the constitutive relation for the electric displacement (Equation 2). Using the constitutive relation we estimate this difference to be around 0.13 GV/m. Secondly, a reduction in the electric field exists due to the geometry induced fringe field.

4. Conclusions

Results are given for the strain and electric field distributions emphasizing the coupled influence of lattice mismatch, piezoelectricity, and spontaneous polarization in an axisymmetrical GaN quantum dot embedded in an AlN matrix. Results indicate that lattice mismatch dominates the resulting field-distribution values, however, in cases with piezoelectricity and spontaneous polarization, violation of inversion symmetry is demonstrated in agreement with the fact that all $\psi$ vector components do not satisfy the same transformation rule. It is important to emphasize that the approach undertaken in this work is general and can be easily applied to any geometry, material combination, and crystal structure. In this 3D work, we confirm that lattice mismatch is the driving force for the overall strain in the case with a GaN quantum dot embedded in an AlN matrix.

Acknowledgment

The authors would like to thank Igor Kornev for helpful discussions.
References
[1] Adel S. Saada, *Elasticity - Theory and Applications*, Pergamon Press Inc. New York, 1974.
[2] Vladimir A. Fonoberov and Alexander A. Balandin. *Journal of Applied Physics*, 94(11):7178-7186, 2003.
[3] Joachim Piprek, *Nitride Semiconductor Devices - Principles and Simulation*, Wiley VHC, 2007.
[4] P. Schnabel *IEEE Transactions on Sonics and Ultrasonics*, Vol. SU-25, NO.1, January 1
[5] L. C. Lew Yan Voon, C. Galeriu, B. Lassen, M. Willatzen, and R. Melnik. *Appl. Phys. Lett.*, 87, 041906 (2005).
[6] M. Willatzen, B. Lassen, L.C. Lew Yan Voon, and R.V.N. Melnik. *Journal of Applied Physics* 100, 024302, 2006.
[7] B. Jogai, J.D. Albrecht and E. Pan, J. Appl. Phy., 94 (10), 6566-6572 (2003).
[8] L. D. Landau, E. M. Lifshitz *Theory of Elasticity*, Course of Theoretical Physics, Volume 7, Pergamon Press, 1970.
[9] D. Bimberg, M. Grundmann and N. N. Ledentsov. *Quantum Dot Heterostructure*, John Wiley and Sons, Chichester, 1999.
[10] O. Stier, M. Grundmann and D. Bimberg *Phys. Rev. B* 59, 5688, 1999.
[11] M. Arlery, J. L. Rouvière, F. Widmann, B. Daudin, and G. Feuillet, H. Mariette. *Appl. Phys. Lett.* 74, 3287 (1999); DOI:10.1063/1.123321
Appendix

\[
L = \left( \frac{\partial}{\partial r} C_{11} \frac{\partial}{\partial r} + C_{11} \frac{\partial}{\partial r} \right) + C_{11} \frac{\partial}{\partial r} C_{13} \frac{\partial}{\partial z} + C_{13} \frac{\partial}{\partial z} C_{44} \frac{\partial}{\partial r} \right) + C_{13} \frac{\partial}{\partial z} C_{33} \frac{\partial}{\partial z} + C_{44} \frac{\partial}{\partial r} \right)
\]