Generalized Plane Piezoelectric Problem: Application to Heterostructure Nanowires

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Introduction

In order to analyze the piezoelectric behavior of materials, it is necessary to solve the coupled mechanical and electrical equations of piezoelectricity. However, the numerical simulations of discretized electro-mechanical equations for 3D systems is in general computationally expensive. Therefore, the disposal of two-dimensional (2D) approaches to problems originally posed in a 3D geometry is always desirable, since they significantly reduce the computing resources and simulation time needed.

In this work we report on a new more general 2D approach called, Generalized plane Piezoelectric (GPP) problem. The approach is based on the idea that for wire-like system with infinite length or high aspect ratios, material properties and external loads being independent of the axial axis x_3, all cross sections along the axial directions are at identical conditions as a result all the strain and electric field components depend only on in-plane coordinates, $\varepsilon_{ij}(x_1,x_2)$ and $E_i(x_1,x_2)$.

Generalized Plane Piezoelectric (GPP) Problem

The equilibrium equations of piezoelectric materials are given by Navier and Poisson equations as:

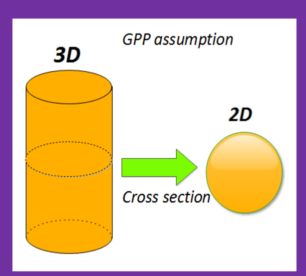
$$\frac{\partial\sigma_{ij}}{\partial x_j} = -f_i\,, \qquad \frac{\partial D_i}{\partial x_i} = \rho\,, \tag{1}$$

Where σ_{ij} is the stress tensor, D_j is dielectric displacements vectors, f_i is body forces and ρ is charge density per unit volume. The fully-coupled constitutive relations for stress and electric displacement are given as [1]:

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} - e_{kij}E_k$$
$$D_i = e_{ikl}\varepsilon_{kl} + \epsilon_{ij}E_k \tag{2}$$

For heterostructure *lattice-mismatched* piezoelectric body containing regions with different elastic constants [$C_{ijkl}(r)$], lattice parameters [$a_k(r)$] and piezoelectric constant [$e_{ikl}(r)$], the Navier and Poisson equations Eq.(1) can be mapped to a standard piezoelectric problem by introducing equivalent lattice-mismatched induced body forces $f_i^{(0)}$ and electric charge density $\rho^{(0)}$ as:

$$f_i^{(0)} = \frac{\partial}{\partial x_j}\left[C_{ijkl}(r)\varepsilon_{kl}^{(0)}(r)\right], \quad \rho^{(0)} = -\frac{\partial}{\partial x_i}\left[e_{ikl}{}^{(l)}\varepsilon_{kl}{}^{(0)}(r)\right], \tag{3}$$



Where the lattice *mis-fit* strain $\varepsilon_{kl}^{(0)}(r)$ is given as:

$$\varepsilon_{kl}^{(0)}(r) = \frac{a_k^{(\mathrm{ref})} - a_k(r)}{a_k(r)}\,\delta_{kl}\,, \tag{4}$$

where $a_k^{(\mathrm{ref})}$ are lattice reference and the total deformation is given as $\varepsilon_{kl}^{(T)}(r) = \varepsilon_{kl}^{(0)}(r) + \varepsilon_{kl}(r)$.

Direct simulation of the above equations for 3D geometry require high computing resource and time. However for wire-like system with infinite length or high aspect ratio all cross sections can be considered to be at identical conditions as a result the strain and electric field components can be expresses as [2].

$$\varepsilon_{ij} = \varepsilon_{ij}(x_1,x_2)\,, \qquad E_i = E_i(x_1,x_2) \tag{5}$$

Then the general displacement solutions of the GPP problem are given as [3] :

$$u_1(x_1,x_2,x_3) = U_1(x_1,x_2) - \frac{A}{2}x_3^2 + \Theta\, x_2x_3\,,$$
$$u_2(x_1,x_2,x_3) = U_2(x_1,x_2) - \frac{B}{2}x_3^2 - \Theta\, x_1x_3\,,$$
$$u_3(x_1,x_2,x_3) = U_3(x_1,x_2) + (Ax_1 + Bx_2 + C)x_3\,, \tag{6}$$
$$\phi(x_1,x_2,x_3) = \boldsymbol{\Phi}(x_1,x_2) + E_0$$

Where U_i are in-plane displacement, A and B show bending strains, C is the axial strain and Θ is angle between transverse and elongation, $\boldsymbol{\Phi}$ (x_1,x_2) is in-plane piezoelectric potential and E_0 is electric field n the axial direction.

The strain and electric field components corresponding to the general solution in Eq.(6) can be expressed as:

$$\varepsilon_{ij} = \varepsilon_{ij}^{(U)} + \varepsilon_{ij}^{(\bullet)}$$
$$E = E^{(\Phi)} + E^{(\bullet)} \tag{7}$$

$$\text{Where } \varepsilon_{ij}^{(U)} \leftrightarrow \begin{pmatrix} \frac{\partial U_1}{\partial x_1} & \frac{1}{2}\left(\frac{\partial U_1}{\partial x_2}+\frac{\partial U_2}{\partial x_1}\right) & \frac{1}{2}\frac{\partial U_3}{\partial x_1} \\ sym. & \frac{\partial U_2}{\partial x_2} & \frac{1}{2}\frac{\partial U_3}{\partial x_2} \\ sym. & sym. & 0 \end{pmatrix},\ \varepsilon_{ij}^{(ABC\Theta)} \leftrightarrow \begin{pmatrix} 0 & 0 & \frac{1}{2}\Theta\, x_2 \\ sym. & 0 & -\frac{1}{2}\Theta\, x_1 \\ sym. & sym. & Ax_1+Bx_2+C \end{pmatrix},\ E^{(\Phi)} = \begin{pmatrix} -\frac{\partial\Phi}{\partial x_1} \\ -\frac{\partial\Phi}{\partial x_2} \\ 0 \end{pmatrix},\ E^{(\bullet)} \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ E_0 \end{pmatrix}$$

Using Eq.(7) the equilibrium equation of Navier and Poisson in Eq. (2) becomes:

$$\frac{\partial}{\partial x_\alpha}\left[\sigma_{i\alpha}^{(U)} + \sigma_{i\alpha}^{(\bullet)}\right] = -f_i\,, \tag{8}$$
$$\frac{\partial}{\partial x_i}\left[D_i^{(\Phi)} + D_i^{(\bullet)}\right] = \rho$$

The set of equations Eq.(5)-(8) with the appropriate boundary conditions define a mathematical 2D problem, where we have to find in-plane displacement $U_i(x_1,x_2)$, piezoelectric potetnial $\boldsymbol{\Phi}$ (x_1,x_2) and constants (A,B,C,Θ,E_0). This problem is here called the ***Generalized Plane Strain (GPP) problem***.

Implementation in COMSOL Multiphysics®

The piezoelectric equilibrium conditions are implemented via the virtual work principle, leading to a weak formulation of Eq. (2), which can be written schematically as[4]:

$$\int_D u_{test}\cdot(\nabla.\sigma + f) = 0, \quad \text{and} \quad \int_D \phi_{test}(\nabla.D - \rho) = 0 \tag{9}$$

Where u_{test} and ϕ_{test} are the test functions for the displacement fields and piezoelectric potential respectively.

Using Eq. (6p, the weak condition (8) becomes:

$$\int_D\left(-\sigma^{(U)}\cdot\varepsilon_{test}^{(U)} + f\cdot U_{test}\right) + surf.\ term1 + \tag{10a}$$
$$\int_D\left(-\sigma^{(\bullet)}\cdot\varepsilon_{test}^{(U)} - \sigma\cdot\varepsilon_{test}^{(\bullet)}\right) = 0$$

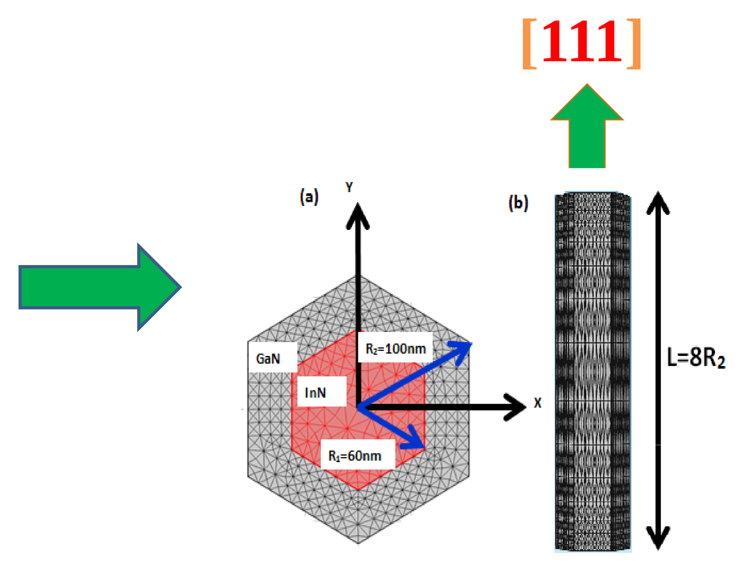
$$\int_D\left(D^{(\phi)}\cdot E_{test}^{(\phi)} + \rho\cdot\Phi_{test}\right) + surf.\ term2\ + \tag{10b}$$
$$\int_D\left(D^{(\phi)}\cdot E^{(\phi)}{}_{test} + D\cdot E_{test}^{(\bullet)}\right) = 0$$

Where $\boldsymbol{\varepsilon}_{test}^{(U)}$ and $\boldsymbol{E}_{test}^{(\bullet)}$ are the test functions. The first integral terms in both Eq. (10a) and Eq. (10b) represent a piezoelectric problem with displacement $U_i(x_1,x_2)$ and piezoelectric potential $\boldsymbol{\phi}(x_1,x_2)$. This problem can be solved by using the 3D application mode on a finite length slice of the original infinitely extended system. The cross section is conveniently meshed. In order to force the dependence on $(\boldsymbol{x_1},\boldsymbol{x_2})$ we use the following trick: We mesh the length of the slice with only one quadrilateral element (what simply doubles the total number of elements used to mesh the cross section) and require periodic boundary conditions to connect the top and bottom surfaces of the slice. This trick effectively imposes that the numerical solutions, that is to be interpreted as $\boldsymbol{U_i}$ and $\boldsymbol{\phi}$, do not depend on $\boldsymbol{x_3}$.

Finally, the contributions of strain $\varepsilon^{(\bullet)}$ and electric field $E^{(\bullet)}$ are added into the weak condition Eq.(10). This is implemented in COMSOL by considering the constants (A,B,C,Θ,E_0) as additional degrees of freedom that are constant throughout the cross section and define them as extra unknown "global variables" [4].

Results

⇒ Zincblende InN/GaN core-shell nanowire grown in [111] direction, with InN core, R1 = 60 nm and GaN shell, R2 = 100 nm. The X- and Y-axes are taken along $[\bar{1}10]$ and $[11\bar{2}]$ crystallographic directions, respectively. We assume that the nanowires are free from external tractions , body forces and electric charge. Finally, the elastic problem is solved by means of the FEM method, using a direct 3D ("exact") calculation, with L = 800 nm, and the GPP problem approaches.



➢ **Electric potential distribution by GPP approach**

Mis-fit strain = -9.6%

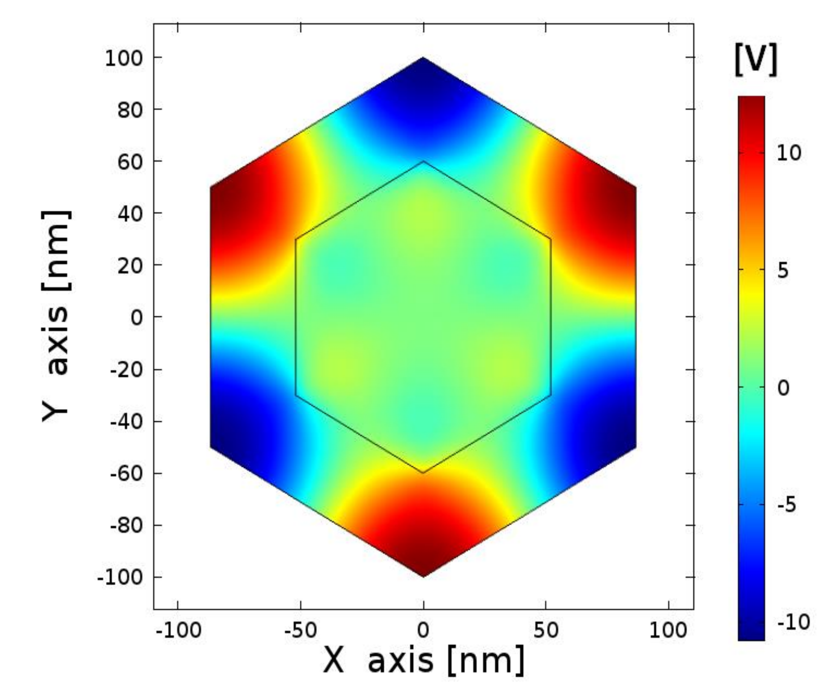


Figure-2 Piezoelectric potential $\boldsymbol{\phi}(x_1,x_2)$ obtained by GPP approach.

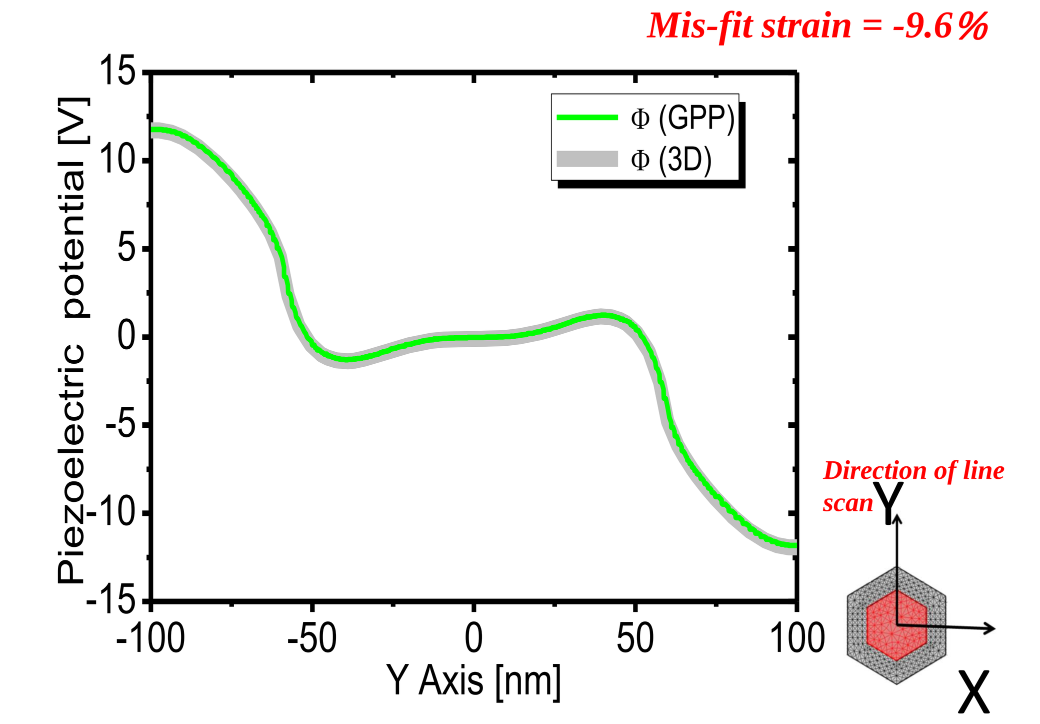


Figure-3. Linescan comparison of Electric potential $\boldsymbol{\phi}$ (x_1,x_2) corresponding to GPP problem and to the central cross section of the finite 3D problem.

- The highest piezoelectric potential is localized inside the GaN with maximum of 11,78V in-plane piezoelectric potential.
- Excellent agreement of piezoelectric potential in both GPP and direct 3D approaches.

➢ **Electric field distributions by GPP approach**

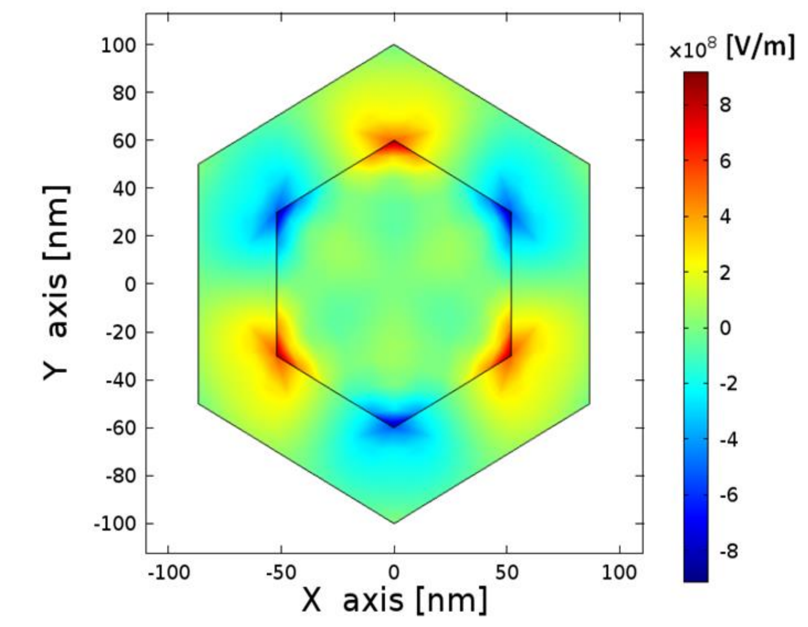


Figure-4 Electric field in the radial direction $E_r(x_1,x_2)$ obtained by GPP approach

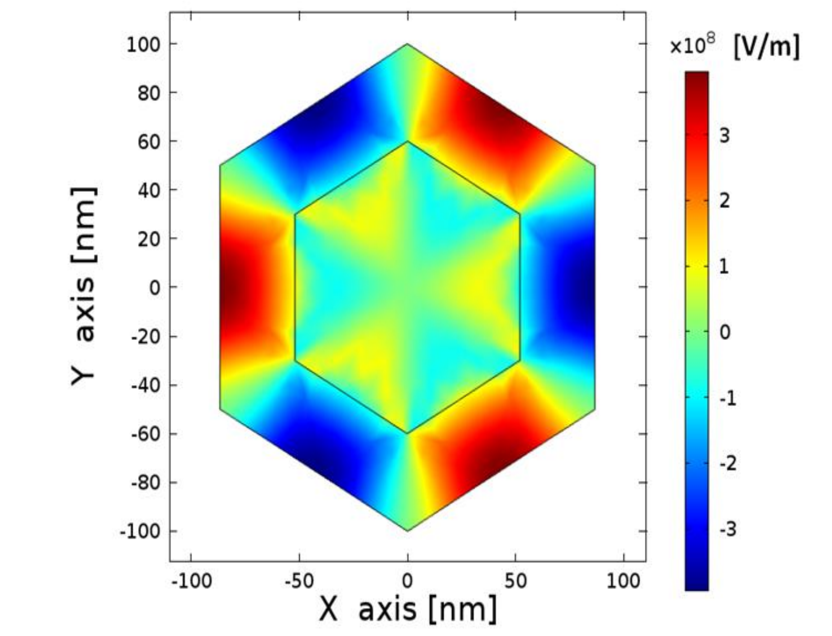


Figure-5 Electric field in the angular direction $E_\phi(x_1,x_2)$ obtained by GPP approach.

- Maximum 925.136 MV/m and 397.417 MV/m in-plane electric field in the radial and angular directions respectively and the electric field in the axial direction corresponds to uniform 136.22 MV/m .

➢ **Electric field: comparison of GPP vs "exact" 3D approaches**

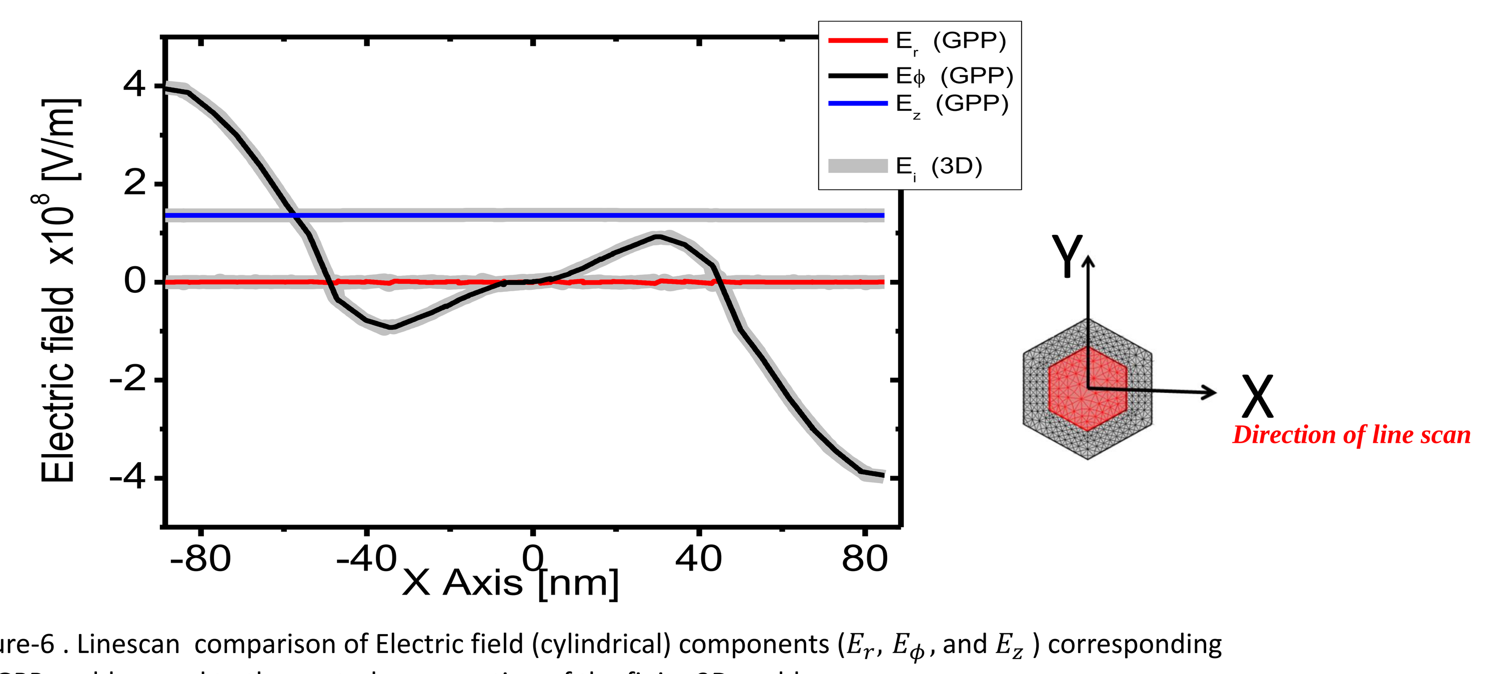


Figure-6 . Linescan comparison of Electric field (cylindrical) components (E_r, E_ϕ, and E_z) corresponding to GPP problem and to the central cross section of the finite 3D problem

- Excellent agreement of electric fields in both GPP and "exact" 3D approaches .

Conclusions

➢ Using GPP problems it has been possible to solve piezoelectric problem in heterostructure nanowires with lesser computing time and less computing resources. The results obtained are also in excellent agreement with results from direct 3D calculations. This prove the versatility of our proposed techniques for obtaining accurate strain and electric fields.

Acknowledgements

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3. Tungyang Chen and Donsen Lai, Proc. R. Soc. Lond. A 453, 2689{2713 (1997).
4. See the Structural Mechanics Module User'sGuide for more details.