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 electromechanical equations for 3D systems is in general computationally expensive. Therefore, the disposal of two-dimensional (2D) approach problems originally posed its 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 systems 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 direction are at identical conditions as a result. The strain and electric field components depend only on the in-plane coordinates $x_1(x_2, x_3)$ and $x_2(x_1, x_3)$.

The highest piezoelectric potential is localized as $\phi = \bar{\phi} + r \phi_r$, where $\bar{\phi}$ is the electric potential and $\phi_r$ represents the local deformation energy. Then the general displacement solutions of the GPP problem are given as [3]:

$$u_1(x_1, x_2) = f_1(x_1) + f_2(x_2), \quad u_2(x_1, x_2) = f_3(x_1) + f_4(x_2).$$

Where $u_1$ and $u_2$ are the test functions for the displacement fields and piezoelectric potential respectively. Using Eq. (6) the electric potential of Navier and Poisson in Eq. (3) becomes:

$$\bar{\phi}(x_1, x_2) = -\int_{x_2}^{x_2+dx_2} f_1(x_1) dx_1 + \int_{x_3}^{x_3+dx_3} f_3(x_1) dx_1.$$

The set of equations Eq.(5)-(6) with the appropriate boundary conditions define a mathematical 2D problem where we have to find in-plane displacement $u_1(x_1, x_2), u_2(x_2, x_3)$ of piezoelectric potential $\phi(x_1, x_2)$ and constant $x_3 \in [a, b]$. This problem is here called the Generalized Plane Strain (GPP) problem.

Implementation in COMSOL Multiphysics®

The piezoelectric equivalent equations are solved using the Vector work principle, leading to a weak formulation of Eq. (3), which can be written schematically as:

$$\int_{x_3}^{x_3+dx_3} f_1(x_1) \Delta \bar{\phi} dx_1 = 0, \quad \int_{x_2}^{x_2+dx_2} f_3(x_1) \Delta \bar{\phi} dx_1 = 0.$$

Where $\Delta \bar{\phi}$, and $\Delta \phi$ are the test functions. The set of Eqs. (4) can be solved using the 3D application mode on a finite length slice of the original infinitely extended system. The cross section is continuously loaded to the voltage via the in-plane direction $u_2(x_1, x_2)$ and $\phi_0(x_1, x_2)$.

Results

- Zincblende InNGaN core-shell nanowire grown in [111] direction, with InN core, $R_1 = 60 \text{ nm}$ and GaN shell, $R_2 = 100 \text{ nm}$. The X- and Y-axes are taken along [110] and [112] crystallographic directions, respectively.
- Electric potential is obtained by means of the FEM method, using a direct 3D ("exact") formulation calculation, with $L = 800 \text{ nm}$, and the GPP problem approaches.
- Excellent agreement of piezoelectric potential in both GPP and direct 3D approaches.

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

- 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: distribution by GPP approach

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

Conclusions

- Using GPP problems is 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.

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References
