Generalized Plane Piezoelectric Problem: Application to Heterostructure Nanowires

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Abstract

The possibility to dispose of two-dimensional (2D) approaches to problems originally posed in a three-dimensional (3D) geometry is always desirable since it reduces significantly the computing resources needed for numerical studies. In this work we report on a new 2D approach called Generalized Plane Piezoelectric (GPP) problem [1] and apply it to the calculation of the strain and electric fields in heterostructure (core-shell) nanowires. The approach is based on the idea that for systems with infinite length or with large aspect ratio, all the cross sections can be considered to be at identical conditions, and hence the strain and electric fields depend only on in-plane coordinates (x_1,x_2) [2]. The GPP approach is able to accommodate piezoelectric problems with any cross-section geometry, symmetry and a wide range of compatible boundary conditions. Therefore, it is well suited to treat piezoelectric problems in nanowires of any material type under different kinds of externally applied constraints or stresses and imposed potentials or surface charges.

As an illustration of the potential applications of the GPP approach, we present a study of the piezoelectric problem in a lattice mismatched zincblende InN/GaN core-shell nanowire with axis along the [111] crystallographic direction. The numerical calculations of GPP are performed on a discretized form of the GPP problem in the framework of continuum piezomechanics by using COMSOL Multiphysics® software. When compared with results of the equivalent problem solved by direct 3D calculations, our 2D calculations exhibit an excellent agreement. This agreement shows the reliability of the GPP approach to obtain efficiently accurate strain, electric and potential distributions for wire-like systems.

This work has been financially supported by the European Union through the Grant Agreement No.265073-NANOWIRING of the Seventh Framework Program, and by the Ministry of Finances and Competitiveness (MINECO) of Spain through Grants CSD2010- 00044 of the Programme "Consolider Ingenio 2010" and MAT2012-33483.

Reference

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