Piezoelectric Fields in Quantum Wires

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INTRODUCTION

There is currently great interest in nanodevices based on nanoscale piezoelectric components. In view of this interest, this article provides a detailed treatment of the piezoelectric effect in zincblende and wurtzite nanowires based on the full piezoelectric tensor for ZnO, GaN and AlN. The theoretical approach used here is based on the continuum model [1-2]. Theoretical results also include comparisons of piezoelectric potentials in wurtzite and zincblende nanowires which will serve as a guide for the proper design of future nanostructures.

THEORY

In this work, the piezoelectric potential is calculated from the piezoelectric polarization, \overline{P} in terms of the strain, \overline{S} and the piezoelectric tensor \overline{e} ; this piezoelectric potential is induced in the nanowire as given by the following relations:

$$\overline{e} = \begin{pmatrix} 0 & 0 & 0 & 0 & e_{x5} & 0\\ 0 & 0 & 0 & e_{x5} & 0 & 0\\ e_{z1} & e_{z1} & e_{z5} & 0 & 0 & 0 \end{pmatrix}$$
for wurtzites

$$\overline{e} = \begin{pmatrix} 0 & 0 & 0 & e_{x4} & 0 & 0 \\ 0 & 0 & 0 & 0 & e_{x4} & 0 \\ 0 & 0 & 0 & 0 & 0 & e_{x4} \end{pmatrix}$$
for zincblendes.

$$\overline{P} = \overline{e} \cdot \overline{S}$$
$$V = -\frac{1}{\varepsilon - \varepsilon_0} \int \overline{P} \cdot d\overline{\rho}$$

RESULTS AND DISCUSSION

In order to cast the piezoelectric stress tensors into more suitable form for cylindrical nanowires, it is necessary to transform from the cartesian coordinate system to the cylindrical coordinate system. This was accomplished using the coordinate transformation matrix [3]. Figures 1 and 2 show the piezoelectric potential distribution as a function of strain applied along z-axis for 50 nm thick and 600 nm long (a) AlN (b) ZnO and (c) GaN nanowires with wurtzite and zincblende crystal structure, respectively, for phonon propagation at an angle η = 90⁰ and with 0.1% strain generated along z-axis. Figures 3 and 4 show the piezoelectric potential distribution as a function of strain applied radially for 50 nm thick and 600 nm long (a) AlN (b) ZnO and (c) GaN nanowires with wurtzite and zincblende crystal structures, respectively. The nanowires are bent such that there is 0.1% strain generated along z-axis. In both cases, the phonon propagation is at an angle η = 0⁰.

CONCLUSION

In view of the great interest in nanodevices based on nanoscale piezoelectric components, this article provides a detailed treatment of the piezoelectric effect in zincblende and wurtzite nanowires based on the full piezoelectric tensor. Knowledge of the full-tensor treatment of this work appears to be especially relevant since many recent experimental efforts do not select the crystal orientations of piezoelectric components to maximize the piezoelectric effect [4,5].

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Fig. 1. Piezoelectric potential distribution for phonon propagation at an angle $\eta = 90^{\circ}$ for wurtzite structures.



Fig. 2. Piezoelectric potential distribution for phonon propagation at an angle $\eta = 90^{\circ}$ for zincblende structures.



Fig. 3. Piezoelectric potential distribution for phonon propagation at an angle $\eta = 0^0$ for wurtzite structures.



Fig. 4. Piezoelectric potential distribution for phonon propagation at an angle $\eta = 0^0$ for zincblende structures.