Piezoelectric Fields in Quantum Wires

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***Abstract*—The piezoelectric effect in zincblende and wurtzite nanowires based on the full piezoelectric tensor following the continuum model has been studied analytically. Theoretical results present comparisons between piezoelectric potentials generated in wurtzite and zincblende nanowires which will serve as a guide for the proper design of future nanostructures in order to achieve maximum piezo-energy.**

I. 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.

II. Theory

In this work, the piezoelectric potential is calculated from the piezoelectric polarization, in terms of the strain, and the piezoelectric tensor which depends on the characteristics of the material and its crystal orientation. The piezoelectric polarization in terms of the piezoelectric tensor and the strain vector is given as

$$\overline{P} = \overline{e} \bullet \overline{S} \tag{1}$$

The piezoelectric tensors for the semiconductor wires with wurtzite and zincblende crystal structures in cartesian coordinate system are respectively given as

$$\overline{e_{wz}} = \begin{pmatrix} 0 & 0 & 0 & 0 & e_{x5} & 0 \\ 0 & 0 & 0 & e_{x5} & 0 & 0 \\ e_{z1} & e_{z1} & e_{z3} & 0 & 0 & 0 \end{pmatrix} \tag{2}$$

$$\overline{e_{zb}} = \begin{pmatrix} 0 & 0 & 0 & e_{x4} & 0 & 0 \\ 0 & 0 & 0 & 0 & e_{x4} & 0 \\ 0 & 0 & 0 & 0 & 0 & e_{x4} \end{pmatrix} \tag{3}$$

and the six component strain vector in cartesian coordinate system is given as

$$\overline{S} = \begin{pmatrix} S_{xx} \\ S_{yy} \\ S_{zz} \\ S_{yz} \\ S_{xz} \\ S_{xy} \end{pmatrix}$$

with the strain components

$$\begin{aligned} S_{xx} &= \frac{\partial u_x}{\partial x}, \quad S_{yy} = \frac{\partial u_y}{\partial y} \\ S_{zz} &= \frac{\partial u_z}{\partial z}, \quad S_{yz} = \frac{1}{2}\left(\frac{\partial u_z}{\partial y} + \frac{\partial u_y}{\partial z}\right) \\ S_{xz} &= \frac{1}{2}\left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x}\right), \quad S_{xy} = \frac{1}{2}\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right) \end{aligned}$$

with u being the acoustic phonon displacement [1], [3].

Now considering a phonon propagating in an arbitary direction η in XZ-plane, the piezoelectric tensor should undergo a rotation transformation by an angle η about the z-axis. In order to cast $\overline{e}$ into a more suitable form for cylindrical quantum wires, we made a transformation from the cartesian coordinate system to the cylindrical coordinate system. Therefore the piezoelectric stress tensor for wurtzite and zincblende quantum wires for phonon propagation at an arbitary angle η in XZ-plane in cylindrical polar coordinate system transforms as

$$\overline{e''} = [a'] \left[[a] \left[\overline{e}\right] \left[\tilde{M}\right] \right] \left[\tilde{M'}\right] \tag{4}$$

where the rotation transformation matrices $[a]$ and $[a']$ are respectively given as

$$[a] = \begin{pmatrix} \cos\eta & 0 & -\sin\eta \\ 0 & 0 & 1 \\ \sin\eta & 0 & \cos\eta \end{pmatrix}$$

$$[a'] = \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and $[M]$ amd $[M']$ are the respective Bond Stress transformation matrices derived from $[a]$ and $[a']$.

In general, the electric displacement vector is given by

$$\overline{D} = \epsilon_0 \overline{E} + \overline{P} = \epsilon \overline{E} \tag{5}$$

Therefore for the case of no free charge in the nanowire, the piezoelectric potential generated in the nanowire due to the piezoelectric polarization is given by

$$\begin{aligned} V &= -\frac{1}{\epsilon - \epsilon_0}\int \overline{P}\cdot d\overline{\rho} \\ &= -\frac{1}{\epsilon'' - \epsilon_0}\left[\int P_r dr + \int rP_\phi d\phi + \int P_z dz\right] \quad (6) \end{aligned}$$

III. Results and Discussion

The most popular and practicable device designs for piezoelectric energy harvesting are the stack structure where the strain is applied vertically and the cantilever approach where the strain is applied radially. In the first case, where the strain is applied along the z-axis of the nanowire, $\frac{\partial u_z}{\partial z}$ is the only dominant component of the strain. Neglecting the strain components in all other directions, the three components of piezoelectrically induced polarization in cylindrical polar co-ordinates for nanowires with wurtzite crystal structure and zincblende crystal structure respectively reduces to

$$\begin{aligned} P_{wz_{r_{zz}}} &= \cos\phi\left(-e_{z1}\sin^3\eta - e_{z3}\cos^2\eta\sin\eta \right. \\ &\quad \left. + e_{x5}\cos\eta\sin 2\eta\right)\frac{\partial u_z}{\partial z} \\ P_{wz_{\phi_{zz}}} &= \sin\phi\left(e_{z1}\sin^3\eta + e_{z3}\cos^2\eta\sin\eta \right. \\ &\quad \left. - e_{x5}\cos\eta\sin 2\eta\right)\frac{\partial u_z}{\partial z} \\ P_{wz_{z_{zz}}} &= \left(e_{z1}\cos\eta\sin^2\eta + e_{z3}\cos^3\eta \right. \\ &\quad \left. + e_{x5}\sin\eta\sin 2\eta\right)\frac{\partial u_z}{\partial z} \\ P_{zb_{r_{zz}}} &= e_{x4}\sin 2\eta\sin\phi\frac{\partial u_z}{\partial z} \\ P_{zb_{\phi_{zz}}} &= e_{x4}\sin 2\eta\cos\phi\frac{\partial u_z}{\partial z} \\ P_{zb_{z_{zz}}} &= 0 \end{aligned}$$

Therefore the piezoelectric potential generated across the nanowire for $\frac{\partial u_z}{\partial z}$ being the only non-zero strain in cylindrical polar co-ordinates is given by

$$V_{zz} = -\frac{1}{\epsilon'' - \epsilon_0}\left[\int P_{r_{zz}} dr + \int rP_{\phi_{zz}} d\phi + \int P_{z_{zz}} dz\right]$$

Figure 1 shows 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 respectively with (i) wurtzite and (ii) zincblende crystal structures for phonon propagation at an angle $\eta = 90^0$ and with 0.1% strain generated along z-axis. The piezoelectric potential generated on stretching 50 nm thick and 600 nm long AlN, ZnO and GaN wurtzite and zincblende nanowires such that 0.1% strain is generated along z-axis with wurtzite and zincblende crystal structures are listed in Table I. The material parameters for the semiconductor wires with wurtzite and zincblende crystal structures have been collected from different literatures [4], [5]. In case of nanowires with wurtzite crystal structure, AlN and ZnO nanowires are found to be superior to GaN nanowires. For the zincblende semiconductor wires, highest piezoelectric potential is obtained from ZnO nanowires in comparison to AlN and GaN nanowires of similar dimension and being subject to similar strain for phonon propagation at $\eta = 45^0$. For phonon prapagation direction parallel or perpendicular to z-axis, zero piezo-energy will be generated from zincblende semiconductor nanowires.

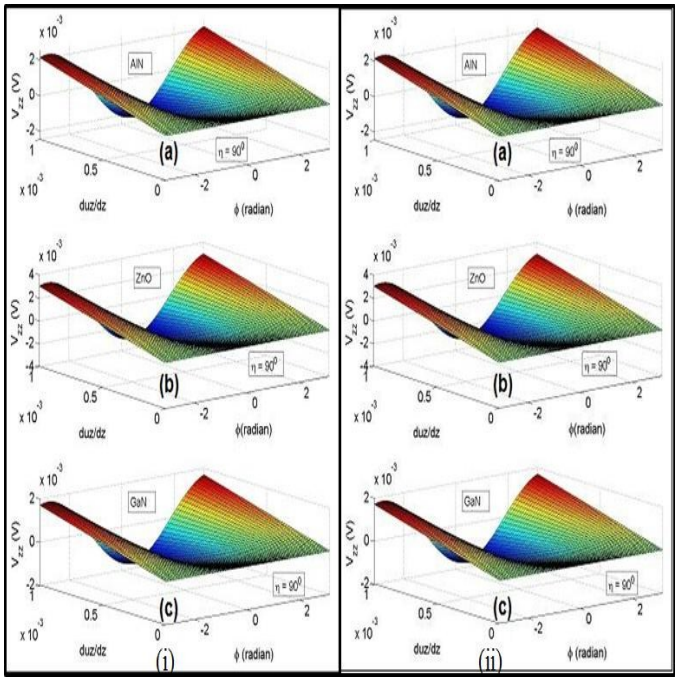

Fig. 1. Piezoelectric potential distribution on stretching 50 nm thick and 600 nm long semiconductor nanowires such that 0.1% strain is generated along z-axis for phonon propagation at an angle $\eta = 90^0$ with (i) wurtzite and (ii) zincblende crystal structures.

TABLE I
Piezoelectric potential generated for 50 nm thick and 600 nm long semiconductor nanowires on streching the wires such that 0.1% stain is generated along z-axis.

Strain (0.1% along c-axis)	Stretching $\lvert V_{zz}\rvert$ (V)					
	Wurtzite			Zincblende		
	AlN	ZnO	GaN	AlN	ZnO	GaN
$\eta = 0^0$	15.1	11.3	4.9	0	0	0
$\eta = 45^0$	2.8	3.7	2	1.3	1.9	1.1
$\eta = 90^0$	3	2.6	1.2	0	0	0

Now considering the cantilever approach, $\frac{\partial u_r}{\partial z}$ is the dominant component of strain. Neglecting the strain components in all other directions, the three components of piezoelectrically induced polarization in cylindrical polar coordinates reduces to

$$
\begin{aligned}
P_{wz_{r_{rz}}} &= \left(e_{x5}\cos\eta\sin^2\phi + \left(-e_{z1}\frac{\sin\eta\sin 2\eta}{2}\right.\right. \\
&\left.\left. + e_{z3}\frac{\sin\eta\sin 2\eta}{2} + e_{x5}\cos\eta\cos 2\eta\right)\cos^2\phi\right)\frac{\partial u_r}{\partial z} \\
P_{wz_{\phi_{rz}}} &= \left(e_{x5}\cos\eta\frac{\sin 2\phi}{2} - \left(-e_{z1}\frac{\sin\eta\sin 2\eta}{2}\right.\right. \\
&\left.\left. + e_{z3}\frac{\sin\eta\sin 2\eta}{2} + e_{x5}\cos\eta\cos 2\eta\right)\frac{\sin 2\phi}{2}\right)\frac{\partial u_r}{\partial z} \\
P_{wz_{z_{zz}}} &= \left(e_{z1}\frac{\cos\eta\sin 2\eta}{2} - e_{z3}\frac{\cos\eta\sin 2\eta}{2}\right. \\
&\left. + e_{x5}\sin\eta\cos 2\eta)\cos\phi\frac{\partial u_r}{\partial z}\right. \\
P_{zb_{r_{rz}}} &= e_{x4}\cos 2\eta\sin 2\phi\frac{\partial u_r}{\partial z} \\
P_{zb_{\phi_{rz}}} &= e_{x4}\cos 2\eta\cos 2\phi\frac{\partial u_r}{\partial z} \\
P_{zb_{z_{rz}}} &= e_{x4}\sin 2\eta\sin\phi\frac{\partial u_r}{\partial z}
\end{aligned}
$$

Therefore the piezoelectric potential generated across the nanowire for $\frac{\partial u_r}{\partial z}$ being the only non-zero strain in cylindrical polar co-ordinates is given by

$$
V_{rz} = -\frac{1}{\epsilon'' - \epsilon_0}\left[\int P_{r_{rz}}dr + \int rP_{\phi_{rz}}d\phi + \int P_{z_{rz}}dz\right]
$$

Figure 2 shows 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 nanowire respectively with (i) wurtzite and (ii) zincblende crystal structures, for phonon propagation at an angle of $\eta = 0^0$. The nanowires are bent such that there is 0.1% strain generated along z-axis.

TABLE II
PIEZOELECTRIC POTENTIAL GENERATED FOR 50 NM THICK AND 600 NM LONG SEMICONDUCTOR NANOWIRES ON BENDING THE WIRES SUCH THAT 0.1% STAIN IS GENERATED ALONG Z-AXIS.

Strain (0.1% along c-axis)	Bending $\lvert V_{rz}\rvert$ (V)					
	Wurtzite			Zincblende		
	AlN	ZnO	GaN	AlN	ZnO	GaN
$\eta = 0^0$	0.41	0.41	0.21	1.3	1.9	1.1
$\eta = 45^0$	6.0	4.5	2.1	0	0	0
$\eta = 90^0$	4.9	4.9	2.5	1.3	1.9	1.1

The piezoelectric potential generated on application of mechanical strain radially to 50 nm thick and 600 nm long AlN, ZnO and GaN wurtzite and zincblende nanowires are listed in Table II. In case of nanowires with wurtzite crystal structure, even on bending the nanowires, AlN and ZnO nanowires are found to be superior to GaN nanowires. For the zincblende semiconductor wires, highest piezoelectric potential is obtained from ZnO nanowires in comparison to AlN and GaN nanowires of similar dimension and being subject to similar strain.Again higher piezoelectric potential is generated on bending the zincblende wires for phonon propagation either parallel or perpendicular to z-axis. For phonon propagation

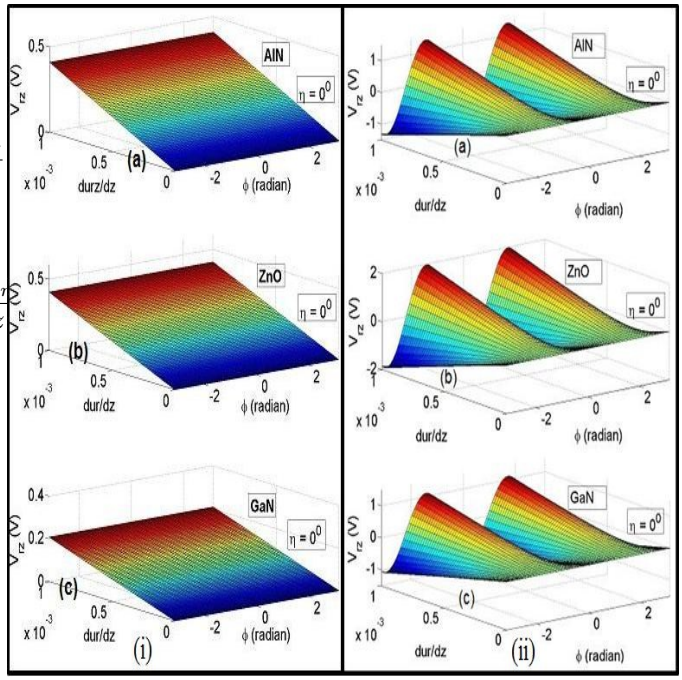

Fig. 2. Piezoelectric potential distribution on bending 50nm thick and 600nm long semiconductor nanowires such that 0.1% strain is generated along z-axis for phonon propagation at an angle $\eta = 0^0$ for (i) wurtzite and (ii) zincblende crystal structures.

at an angle 45^0 with respect to z-axis, zero piezo-energy is generated on bending the zincblende nanowires. Even though the semiconductor nanowires with wurtzite crystal structure generate higher piezoelectric potential in contrast to zincblende crystal structure, in practice wires with zincblende structures may be more practical because bending mode is easier to realize than stable compressional modes [4]. In this paper we have estimated the piezoelectrically induced electric potential distribution in wurtzite and zincblende AlN, ZnO and GaN nanowires for the zero free-charge case. With the presence of free charge in the nanowires, there will be electron-phonon as well as hole-phonon interactions and the net output voltage generated will be affected by this phonon scattering which is beyond the scope of this analytical treatment. This full-tensor treatment appears to be especially relevant since many recent experimental efforts do not appear to select the crystal orientations of piezoelectric components to maximize the piezoelectric effect [6], [7].

IV. 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 [6], [7].

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