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Potential distribution in deformed ZnO nanowires

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Abstract

The potential distribution in a deformed ZnO nanowire relies upon its piezoelectric and semiconductive properties. Here we systematically investigate the influence of different parameters on the equilibrium potential distribution. In particular we calculate the electric potential distribution when thermodynamic equilibrium among free charge carriers is achieved for nanowires under different doping concentrations (n or p type), different applied forces, and different geometric configurations. We show that doping concentration is the parameter that mostly affects the magnitude and distribution of the piezoelectric potential.

Keywords: Nanowire; ZnO; Nanogenerator

1. Introduction

Nano-devices for energy harvesting may become critical components of self-powered nanodevices for different applications such as implantable microsystems for medical applications and for nodes of wireless sensors networks. Piezoelectricity is a very promising method to harvest mechanical energy from the environment. Body movement, muscle stretching, acoustic waves and blood flow can all be sources of mechanical energy, that can be converted into electricity by means of the piezoelectric effect.

Piezoelectric nanogenerators using nanowires (NWs) have been recently demonstrated for converting nanoscale mechanical energy into electricity[1,2]. The principle of nanogenerators is that an applied external force exerted at the top of the ZnO nanowire generates a piezoelectric potential due to elastic deformations. The resulting potential can drive the flow of charge carriers through an external load. The flowing direction of charge carriers is controlled by the Schottky barrier formed at the junction of the nanowire with an external electrode.

A continuum model for the electrostatic potential in a bent piezoelectric nanowire has been presented[3] and applied to a variety of piezoelectric nanowires and nanowalls[4]. This model and its calculations were based on the Lippman theory[5], which can be employed when the doping concentration is extremely low, thus allowing to neglect the electrical conductivity of the material. By applying those calculations to a deformed nanowire, it has been demonstrated that the compressed side of the NW exhibits a negative potential, while the stretched side presents a

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positive potential. The voltage drop created across the section of the nanowire when it is laterally deflected, is at the base of the nanogenerator theory.

A new model, including the statistics of electron/holes, has been presented[6] in order to obtain a more accurate estimation of the piezoelectric potential in deflected nanowires with moderate conductivity (i.e. normal doping range). The same model has been used[7] in order to investigate the influence of various parameters on the electric potential distribution in a laterally bent semiconductive nanowire. Previous works[3,4,6] only considered n-type doping, because as-grown ZnO nanowires are typically n-type; the piezoelectric potential of deflected p-type nanowires has been shown[8] for a certain doping concentration; here we show how the electrical potential distribution depends on applied force, geometric parameters, and doping (including various p-type doping concentrations).

Calculations[6] take into account both the piezoelectric constitutive equation and the redistribution of electrons under thermodynamic equilibrium (Fermi-Dirac statistics).

2. Calculations and Results

The Finite Element Method (FEM) was used to solve the nonlinear partial differential equations describing the piezoelectric constitutive equation and the redistribution of electron under thermodynamic equilibrium. A ZnO nanowire, epitaxially grown along the c axis, is laterally bent by a force exerted at the top.

The material constants for ZnO used in the calculations are chosen as follows[6]: Young’s modulus E=129 GPa; Poisson’s ratio ν=0.349; relative dielectric constants κ_∞=7.77, $\kappa_{||}$= 8.91; piezoelectric constants e_{31}= -0.51 C/m^2, e_{33}= 1.22 C/m^2, e_{15}= -0.45 C/m^2; other physical parameters are adopted from Gao et al.[6]

The nanowire is modeled as a cylinder and the force is uniformly applied at the top surface of the nanowire, perpendicular to its axis, in order to avoid punctual deformations.

Figure 1a shows the influence of the donor concentration on the equilibrium piezoelectric potential for different donor concentrations between 0.05x10^{17} cm^{-3} and 5x10^{17} cm^{-3}. The length of the nanowire is 600 nm and the radius is 25 nm. The force exerted at the top is 80 nN. The stretched side (y<0) shows a small positive electric potential (as explained before); the compressed side (y>0) instead has a negative potential; the electrons are therefore accumulated in the stretched side (positive potential) so that the stretched side (y<0) is more conductive and, therefore, the voltage difference in this region is smaller than in the (depleted) compressed side (y>0). The positive potential in the stretched side is almost zero for high donor concentration (above 10^{17} cm^{-3}).

Figure 1b shows the same calculation carried out for a p-type nanowire, with acceptor concentration between 0.1x10^{17} cm^{-3} and 5x10^{17} cm^{-3}. In this case, analogously, holes are accumulated in the compressed side (negative potential) so that the compressed side (y<0) is more conductive and, therefore, the voltage difference in this region is smaller than in the (depleted) stretched side (y>0). The negative potential in the compressed side is almost zero for high acceptor concentration (above 10^{17} cm^{-3}).

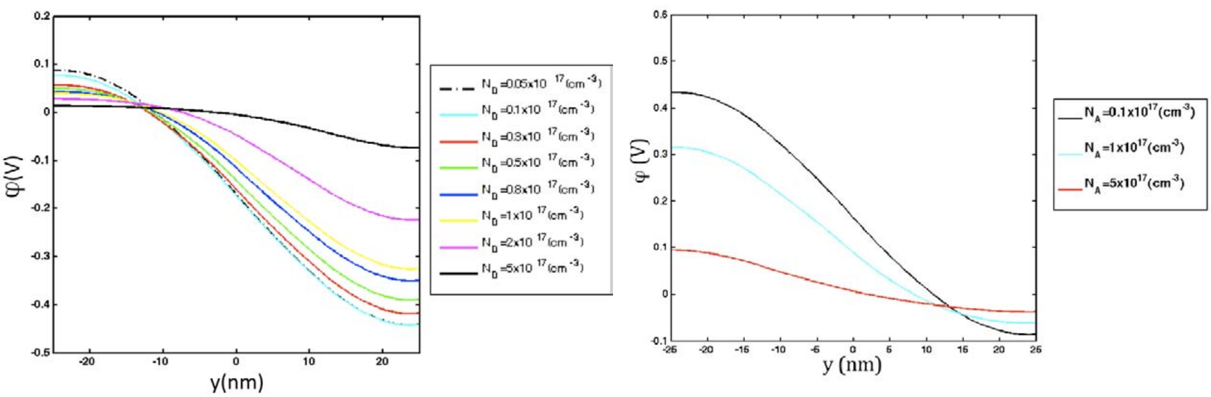

Fig. 1. (a) Piezoelectric potential for different donor concentrations; (b) Piezoelectric potential for different acceptor concentrations.

Figure 2 shows the influence of the applied force on the equilibrium potential. The geometric parameters are the same as before, with donor concentration equal to $N_D=1x10^{17}$ cm^{-3}. The force is increased in the range 40 nN to 140 nN. As explained above, during the simulations, the force was applied at the top surface of the nanowire in order to avoid punctual deformations. When increasing the applied force, the electric potential in the compressed side increases as well.

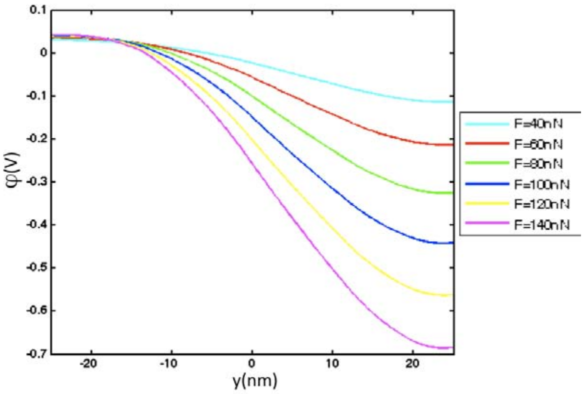

Fig. 2. Piezoelectric potential for different forces exerted at the top of the nanowire.

The influence of geometric parameters of the nanowire on the equilibrium potential is shown in figure 3. Figure 3a shows that the length of the nanowire does not induce changes in the piezoelectric potential. In this case the radius of the nanowire has been kept constant at 25 nm, and the length has been varied in the range 200 nm to 1000 nm. The donor concentration and the applied force have been kept constant at $1x10^{17}$ cm^{-3} and 80nN, respectively.

Figure 3b shows the influence of the radius dimension on the piezoelectric potential, when all other parameters are kept constant. The effect of the variation of the radius has been investigated in the range 25 nm $< a <$ 100 nm. The electric potential is almost neutralized for a radius of 100 nm.

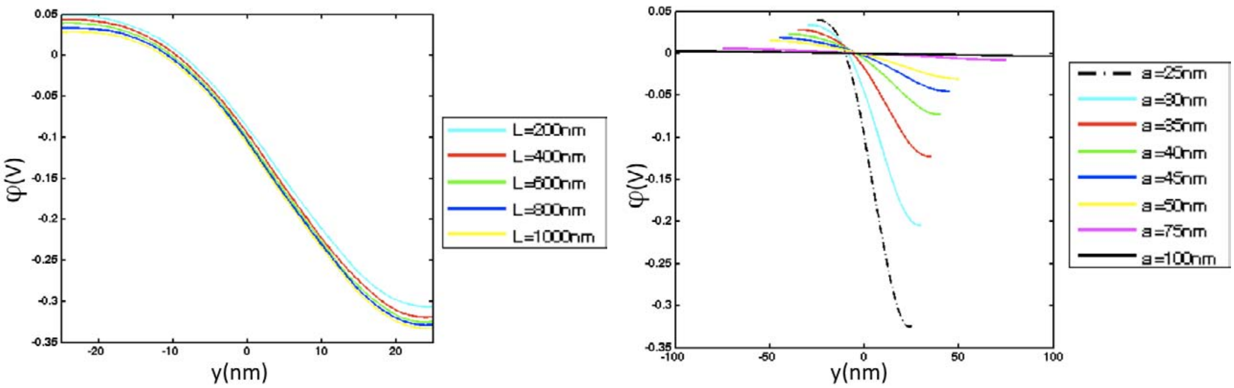

Fig. 3. (a) Piezoelectric potential for different lengths of the nanowire; (b) Piezoelectric potential for different radius dimension of the nanowire.

3. Conclusions

The influence of different parameters on the equilibrium piezoelectric potential distribution in a deformed ZnO nanowire has been systematically investigated. The doping concentration was the parameter most affecting the potential distribution.

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