A Numerical Analysis on the Effect of Piezoelectric Charges on the Surface Depletion Layer of ZnO Nanowires

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INTRODUCTION

One dimensional (1D) nanostructures have attracted much attention in applications including nanoelectronic devices [1], nanogenerators [2] and sensors [3]. In particular, wide-bandgap metal-oxide nanowires (NWs) such as ZnO NWs have been the focus of much research. The application of ZnO NWs, however, requires well defined electrical properties. In this study the perturbation of the surface depletion thickness perturbation of ZnO NWs caused by immobile charges has been investigated.

THEORY

The crystal symmetry of ZnO is responsible for the two different components of the internal polarization, spontaneous polarization and piezoelectric polarization. On application of an external strain to a piezoelectric crystal, a macroscopic polarization is produced as a result of the displacements of ions which can be expressed by the following equation [4].

$$P_i = e_{ijk}.S_{jk} \tag{1}$$

$$e_{ijk} = \begin{pmatrix} 0 & 0 & 0 & 0 & e_{x5} & 0 \\ 0 & 0 & 0 & e_{x5} & 0 & 0 \\ e_{z1} & e_{z2} & e_{z3} & 0 & 0 & 0 \end{pmatrix} \tag{2}$$

where t P_i is the polarization, e_{ijk} is the piezoelectric coefficient constant and S_{jk} is the applied strain. In the depletion region of semiconductor the piezoelectric charges may be added to the ionized impurities (donor or acceptor) causing a change in the depletion depth. The free carriers migrate to maintain quasi-neutrality in the non-depleted region [5].

DISCUSSION

To investigate the change in the depletion region caused by immobile piezoelectric charges, first the depletion region equation in a 1D structure is derived based on the theory proposed by Schmidt *et al.* [6]. Figure 1 is a schematic diagram of ZnO NW and its band diagram energy. The absorbed oxygen on the surface of ZnO NW can be modeled as surface charges (N_s). These surface charges should be balanced by a negative charge to satisfy charge neutrality. The surface charges (N_s) can be expressed as following.

$$N_s = e^2 D_{it} \Psi_s \tag{3}$$

where D_{it} is the interface state density and Ψs is the surface potential. Starting with neutrality condition, the surface depletion width of ZnO NW can be derived as the following [6].

$$\pi(r_{phys}^2 - r_{elec}^2)\rho + 2\pi r_{phys} N_s = 0 \tag{4}$$

$$r_{elec} = \sqrt{r_{phys}^2 - \frac{2 r_{phys} q^2 D_{it} \psi_0}{\rho(1 + \frac{r_{phys} q^2 D_{it}}{2\varepsilon_s})}} \tag{5}$$

The immobile piezoelectric charge density can be expressed as equation 1[5].

$$N_{PE} = -\frac{1}{q}\frac{\partial}{\partial x_i}(e_{ijk}.\frac{\partial u_i}{\partial x_k}) \tag{6}$$

So the charge density in the depletion region is

$$\rho(r) = q[N_v \exp(\frac{-E_g}{KT}) \exp(\frac{-KT}{q}\psi_r) - N_c \exp(\frac{-E_g}{KT}) \exp(\frac{-KT}{q}\psi_r) + N_D - N_A + N_{PE}] \quad (7)$$

The simulation results shown in figure 2 shows that the NWs with smaller radius have larger surface depletion thickness. Figure 3 present the surface depletion perturbation caused by immobile piezoelectric charges for NWs with different radius. Since the electrical and optical properties of ZnO NWs are strongly dependent to the surface depletion region [7] the simulation results show that the induced immobile piezoelectric charges might have an effect on the electrical and optical properties of NWs through the surface depletion perturbation.

CONCLUSION

In summary, the effect of piezoelectric polarization charges on the surface depletion widths of ZnO NWs has been studied. The Numerical calculations show that the immobile piezoelectric charges might change the surface depletion thickness which strongly affects the electrical properties of ZnO NWs.

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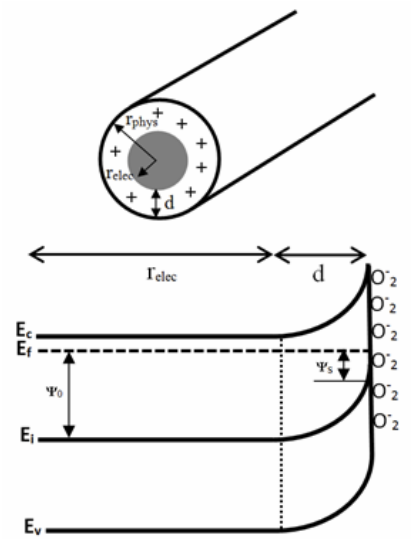

Fig. 1. The schematic diagram of a ZnO NW and its band diagram energy.

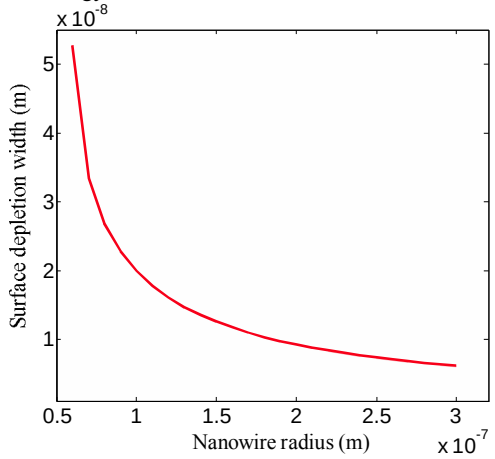

Fig. 2. The surface depletion region of ZnO NW versus the radius.

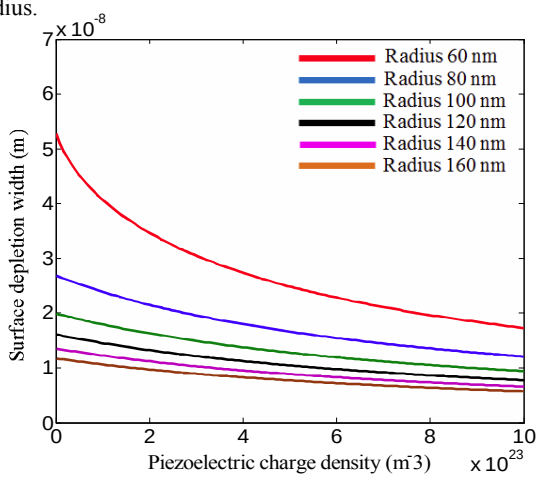

Fig. 3. The surface depletion width of a ZnO NWs (with different radius) in presence of piezoelectric charges.