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

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***Abstract*— We have investigated the effect of piezoelectric charges on the surface depletion region of ZnO NWs. By considering an inner region with a non-negligible density of free carriers and a depleted region at surface of the ZnO NWs and by solving the Poisson equation in the depleted region, the surface depletion width is derived. Thus, the effect of piezoelectric charges on the surface depletion region has been investigated.**

Keywords-component; ZnO Nanowire; piezoelectric charge; depletion region;

I. INTRODUCTION

Compound semiconductors nanostructures such as ZnO nanowires (NWs) and GaN NWs have been the focus of much research due to their unique properties. Compound semiconductors have the key advantages such as the piezoelectric and semiconducting properties. Because of these dual properties, they can be used as a junction device for performing diode and transistor-type functions [1- 4]. These properties make them the promising candidates for applications such as electromechanically coupled sensors and transducers [5]. However, the application of piezoelectric semiconductor nanowires (NWs), requires well defined electrical properties which might be affected by its piezoelectric properties. Here we have investigated the effect of piezoelectric charges on the surface depletion layer of ZnO NWs.

II. THEORY

The compound semiconductors such as ZnO and GaN are belong to non-centrosymmetric crystal groups and the lack of central symmetry in their crystal structure makes them piezoelectric materials. In case of ZnO NWs its crystal symmetry is responsible for the two different components of the internal polarization, spontaneous polarization and piezoelectric polarization. The result of piezoelectric effect is bound charges which can be related to the induced strain by the following equations [6, 7].

$$\begin{aligned} T &= -e.E + c^E : S \\ D &= \varepsilon^S .E + e : S \end{aligned} \tag{1}$$

where T is the stress, c is the elastic stiffness constant, e is the polarization constant, E is the electric field, D is the electric displacement, S is the strain and, □ is the electric permittivity. The result of an external strain to a piezoelectric material is a macroscopic polarization which in case of a wurtzite crystal in Cartesian coordinates can be expressed by the following equation [8].

$$D_i = e_{ijk} . S_{jk} \tag{2}$$

$$e_{ijk} = \begin{pmatrix} 0 & 0 & 0 & 0 & e_{x5} & 0 \\ 0 & 0 & 0 & e_{x5} & 0 & 0 \\ e_{z1} & e_{z2} & e_{z3} & 0 & 0 & 0 \end{pmatrix} \tag{3}$$

However, in case of piezoelectric semiconductors the piezoelectric polarization charges will be screened by free carriers at regions that density of free carriers is not zero and the above equations cannot be employed. Under such condition the generation of the piezoelectric charge might be considered equivalent to the generation of an electrical field or a potential [6]. However, in the depletion region of semiconductor where the density of free carriers is negligible the piezoelectric constitutive equations can be used. In depleted region the piezoelectric charges may be added to the ionized impurities. In the non-depleted region where the density of free carriers is not negligible the free carries migrate to the region where piezoelectric polarization appears to maintain the quasi-neutrality. The migration time of free carries is on the order of the dielectric relaxation time which can be described as the following [9]:

$$\tau_r = \frac{\varepsilon}{\sigma} \tag{4}$$

where E is electric permittivity and σ is the conductivity of material. In case of ZnO NWs which have a density of free electrons around 1018 cm-3 [10], the relaxation time is about one picosecond. Since the piezoelectric polarization charges will be screened by free carriers in the non-depleted region,

the piezoelectric charges have been considered in the depleted region of a single ZnO NW.

III. DEPLETION REGION IN A 1D STRUCTURE

To investigate the depletion region, the perturbation caused by immobile piezoelectric charges, two regions have been considered in the ZnO NW structure. The inner region is a non-depleted region where the density of free carriers is not negligible and the second region is a depleted region which is formed at the surface of NW. In figure 1 the schematic representation of a single nanowire and its band bending in the radial direction are depicted the radius of non-depleted region is r_{elec} and the depletion region width is d. by deriving the surface depletion layer of a single ZnO NW and determining the piezoelectric induced charge density, in terms of equivalent density of charges, the effect of piezoelectric charges on the surface depletion width has been investigated. The depletion region in a 1D structure can be derived based on the theory proposed by Schmidt *et al.* [11]. The surface charges (N_s) should be balanced by a negative depletion charge to satisfy charge neutrality. The surface charge density can be described as following [12]:

$$N_s = e^2 D_{it} \Psi_s \tag{5}$$

where D_{it} is the interface state density, e is the electron charge and ψ_s is the surface potential. By defining the electrostatic potential ψ_r which is the distance between the Fermi level and E_i and by considering the fully ionized donors and acceptors the charge density in the depletion region can be expressed as following [13].

$$\rho(r) = q[N_v \exp(\frac{-E_g}{KT}) \exp(\frac{-KT}{q}\psi_r) - N_c \exp(\frac{-E_g}{KT}) \exp(\frac{-KT}{q}\psi_r) + N_D - N_A] \tag{6}$$

where Nv and Nc are the effective density of states. By solving the Poisson equation in polar coordinates, the electrostatic potential ψr can be obtained.

$$\psi(r) = \psi_o \text{.....} (0 \le r \le r_{relec}) \tag{7}$$

$$\psi(r) = \psi_o - \frac{eN_D}{4\varepsilon}\left(r^2 - (r_{Phys} - d)^2\right) + \frac{eN_D}{2\varepsilon}(r_{Phys} - d)^2 \left(Ln(\frac{r}{r_{Phys} - d}) \right) \text{.....} (r_{elec} \le r \le r_{phys}) \tag{8}$$

where the ψ_0 is the potential at r =0 and the value of the potential ψ_0 can be obtained by setting (1) to zero and solving for $\psi_0 = \psi(0)$. Starting with neutrality condition the surface

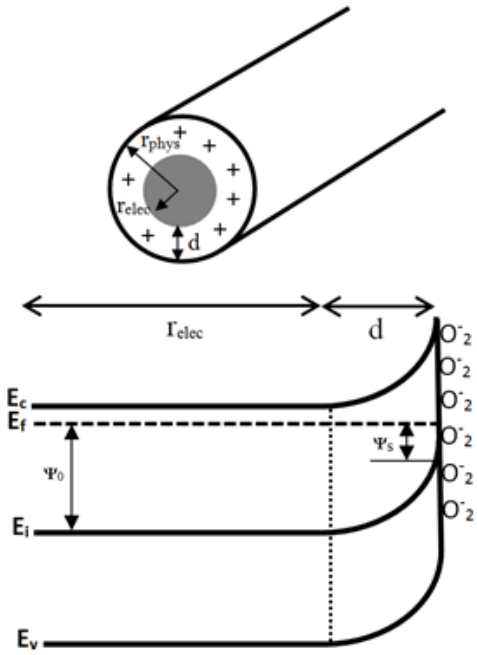

Figure 1. The schematic diagram of a ZnO NW and its band diagram energy.

depletion width (d) in a 1D structure can be derived as the following [11]:

$$\pi(r_{phys}^2 - r_{elec}^2)\rho + 2\pi r_{phys} N_s = 0 \tag{9}$$

$$r_{elec} = \sqrt{r_{phys}^2 - \frac{2 r_{phys} q^2 D_{it} \psi_0}{\rho(1 + \frac{r_{phys} q^2 D_{it}}{2\varepsilon_s})}} \tag{10}$$

$$d = r_{phys} - r_{elec} \tag{11}$$

The piezoelectric induced charge density, in terms of equivalent density of charges can be described as the following [9];

$$N_{PE} = -\frac{1}{q}\frac{\partial}{\partial x_i}(e_{ijk} \cdot \frac{\partial u_i}{\partial x_k}) \tag{12}$$

where, u_i is the vector displacement of ions in the crystal structure of the piezoelectric material. Considering the immobile piezoelectric charge in the depletion region, the charge density in the depleted region can be modified as following.

$$\rho(r) = q[N_v \exp(\frac{-E_g}{KT}) \exp(\frac{-KT}{q}\psi_r) - N_c \exp(\frac{-E_g}{KT}) \exp(\frac{-KT}{q}\psi_r) + N_D - N_A + N_{PE}] \quad (13)$$

The sign of piezoelectric charges is a function of applied stress tensor and dependent on the direction of generated electric filed might be considered as a positive or negative piezoelectric charges. Substituting the values of the respective coefficients from Table I the numerical analyses have been performed.

IV. RESULTS AND DISCUSSION

Figure 2 shows the surface depletion width of ZnO NWs with different radii without considering any induced piezoelectric polarization charges in the surface depletion region. As it is seen in figure 2 the NWs with smaller radius have a larger depletion layer. The surface depletion region perturbation caused by piezoelectric charges can be seen in figure 3 where the surface depletion region of NWs with different radiuses in presence of piezoelectric charge at depletion layer has been illustrated. For more comparison, the normalized depletion widths presented in figure 2 are shown in figure 4 which demonstrate that in the case of the NWs with smaller radius the depletion region perturbation is stronger than for NWs with larger radius. Since the electrical and optical properties of ZnO NWs are strongly dependent to the surface depletion region the simulation results show that the induced immobile piezoelectric charges has an effect on the electrical and optical properties of NWs.

Table 1. Constants used in the numerical analysis.

Material	E_g	N_s	N_D	N_A	ϵ_s
ZnO	3.37[11]	7×10^{13}cm^{-2}[10]	10^{18}cm^{-3}[10]	~0	8.5[12]

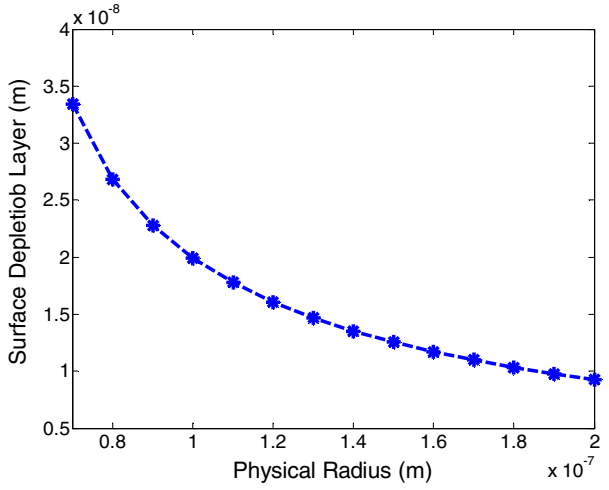

Figure 2. The surface depletion region of ZnO NW versus the physical radius.

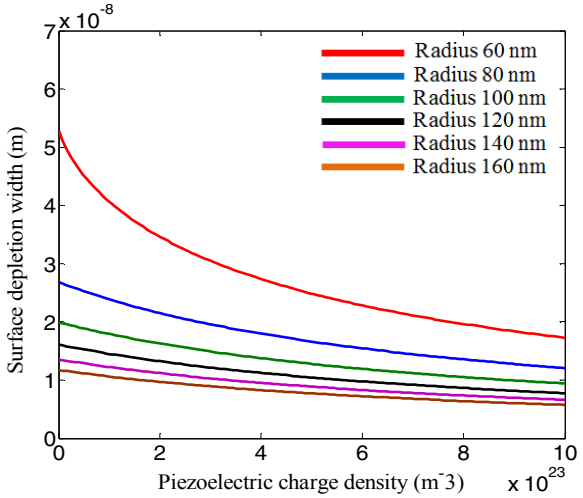

Figure 3. The surface depletion width of a ZnO NWs (with different radius) in presence of piezoelectric charges.

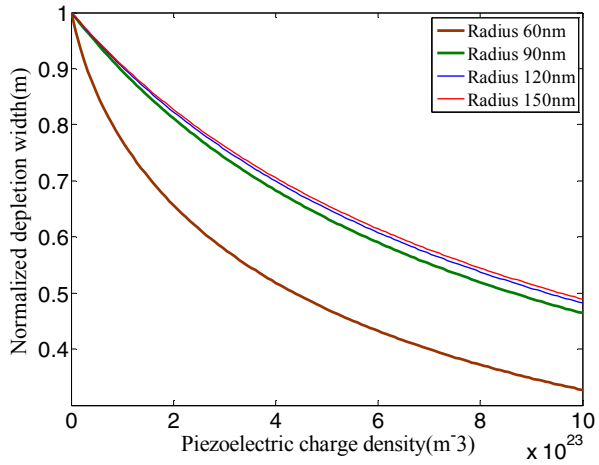

Figure. 4. The normalized surface depletion width of a ZnO NWs (with different radius) in presence of piezoelectric charges.

V. CONCLUSION

The effect of piezoelectric charges on the surface depletion layer of ZnO NWs has been investigated. To this end, two regions were considered in the ZnO NW: a non-depleted region and a depleted region. By solving the Poisson equation in the depleted region, the electrostatic potential and depletion region width have been derived. Considering piezoelectric induced charge density, in terms of equivalent density of charges the numerical analysis shows that the immobile piezoelectric charges cause a change on the surface depletion layer ZnO of nanowire and the changes are more obvious in case of ZnO nanowires with smaller radius.

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