

Monte Carlo Simulation of Submicron ZnO n⁺-n -n⁺ Diode

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ABSTRACT

The steady-state electron transport in ZnO n⁺-n -n⁺ diode with 0.25 μm -long active layer was studied using Monte Carlo simulation. Effect of bias voltage changing and different temperature were calculated on electron distribution, potential, electric field and electron drift velocity as a function of distance between anode and cathode.

Keywords:- Monte Carlo method; active layer; bias voltage.

INTRODUCTION

At the start of the 21st century the wide-band-gap semiconductors (WBS) like ZnO, GaN and SiC (with band-gap 3.43, 3.39 and 3.2 eV, respectively) are on the rise. Between them ZnO has more attraction because it is transparent to visible light in its crystalline form so it has the potential to be the starting material for so-called 'transparent electronics', where the entire device is transparent [1-4]. Here, we simulate submicron ZnO n⁺-n -n⁺ diode because this simulation can provide much useful information on the transport properties of more complex structures [5-6]. On the other hand, submicron structure is one of the most favored devices in the construction of large scale integrated circuits because of simplicity of construction [7].

MODEL DETAILS

In the case of a device simulation the Boltzman transport equation (BTE) has to be solved self-consistently with the Poisson's equation (PE), because the particles are accelerated by the electric field which in turn depends on the particle distribution [6-9].

The ZnO n⁺-n-n⁺ diode is a unipolar one dimensional device that consists of a 0.15 μm wide region with a constant doping of $5 \times 10^{23} \text{ cm}^{-3}$ followed by 0.25 μm of $2 \times 10^{21} \text{ cm}^{-3}$ and again 0.15 μm of $5 \times 10^{23} \text{ cm}^{-3}$ (Fig.1). To simulate this structure, the real space is discretized on a grid of 110 nodes with a constant spacing of 5nm. The Monte Carlo simulations have been performed with about 10^6 particles for more than 40 ns. The PE was solved every 2 fs. The MC simulation includes two valley conduction band model with ionized impurity, polar optical phonon, acoustic deformation and intravalley scattering mechanisms. The parameters used in this MC simulation are shown in table 1.

Material parameters			
Mass density, kgm ⁻³	5600		
Sound velocity, ms ⁻¹	6400		
Static relative permittivity, ε ₀	8.2		
High frequency relative permittivity, ε _∞	3.7		
Acoustic deformation potential, (eV)	14		
Polar optical phonon, ħω _{op} (meV)	72		
Direct energy gap, E _g (eV)	3.43		
Valley parameters			
	Γ	U	K
Electron effective mass (m [*] /m ₀)	0.25	0.4	0.3
Nonparabolicity coficients (eV ⁻¹)	0.312	0.059	0.65
Valley seperation (eV)	0	2.1	2.9
Equivalent valley number	1	6	2

Table 1. Important parameters used in the simulations for ZnO n⁺-n -n⁺. [10].

RESULTS

The free electron density for different bias is shown in Fig. 2. It shows that in absence of any external voltage the electrons diffuse from the high doped regions into the active layer or low doped region. But the dipole of charge at the two interfaces induces a field that prevents this tendency. When the bias voltage increases because of electron injection into the active layer from anode and cathode, free electron density enhances in this region [6]. Fig. 3 shows that when a voltage is applied to the structure, the potential drops mostly inside the active layer. Variation of electric field as function of device length for these bias voltages is shown in Fig. 4. It can be seen when an external voltage is applied a very high electric field is found that reaches a maximum near the anode. It causes carriers that enter the active layer overcoming the small potential barrier at the cathode are accelerated quasi ballistically for about half of the active layer region [6-11]. So the average electron velocity increases up to a maximum. After that due to the electron transfer into the satellite valleys and to backscattering from the anode, drift velocity decreases (Fig. 5).

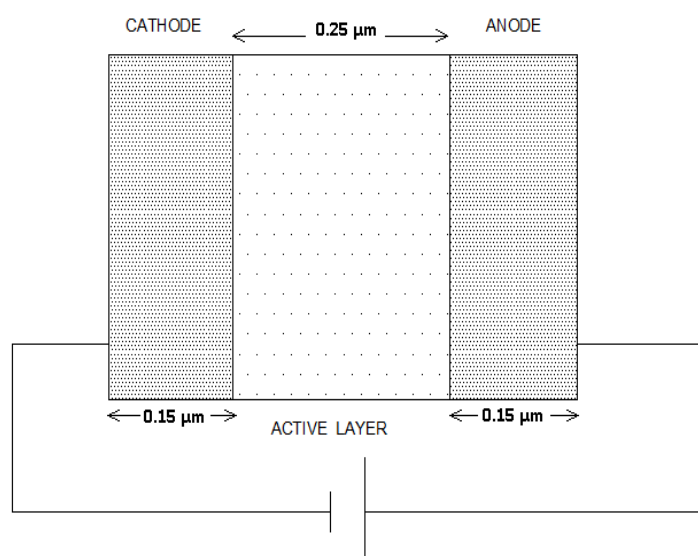


Figure 1. Geometry of n^+-n-n^+ diode.

Fig 6-9 show the temperature effect on above parameter as function of distance for diode with 0.5 applied voltage. Fig. 7 shows that as temperature increases the barrier height of n^+-n junction increases. Also with raising temperature electron drift velocity reduces in the active layer due to enhanced scattering (Fig. 9).

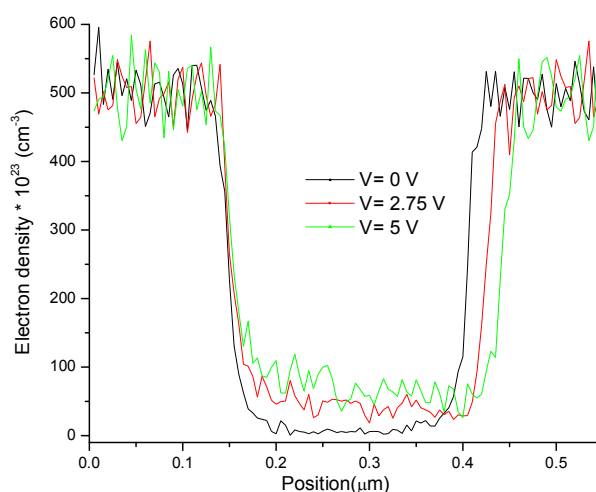


Figure 2. Distribution of electron density along ZnO n^+-n-n^+ diode under different bias voltages.

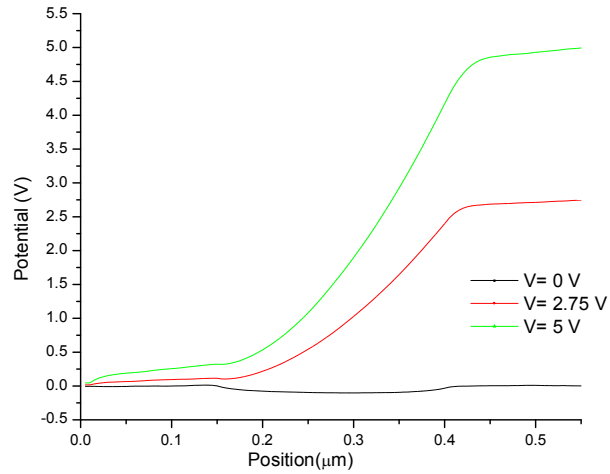


Figure 3. Electrical potential along ZnO $n^+ - n^-$ diode under different bias voltages.

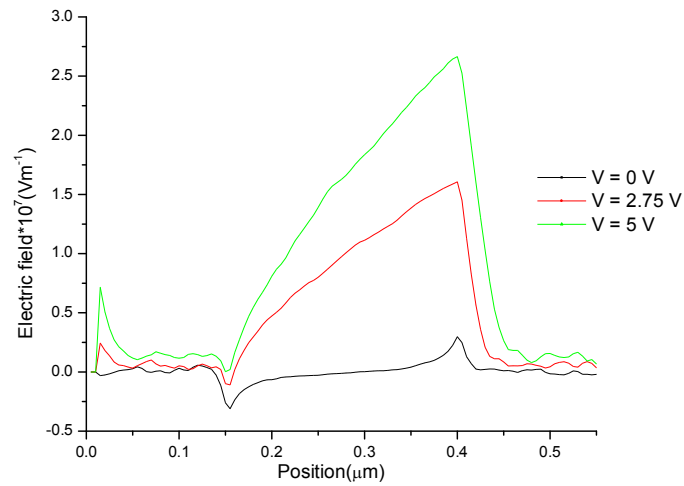


Figure 4. Electric field along ZnO $n^+ - n^-$ diode under different bias voltages.

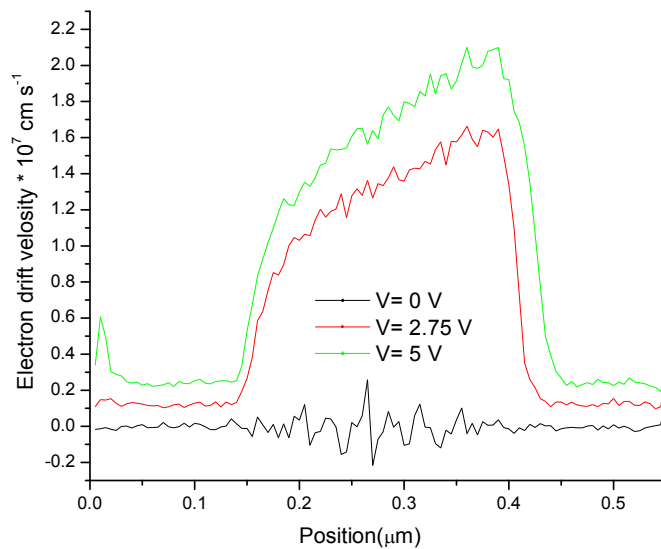


Figure 5. Electron velocity along ZnO $n^+ - n^-$ diode under different bias voltages.

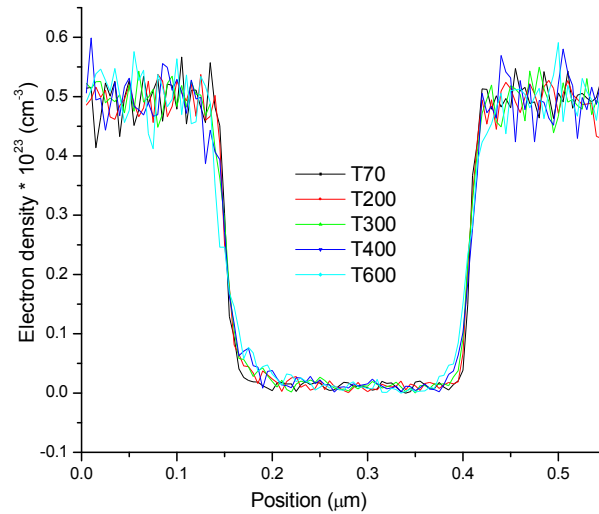


Figure 6. Distribution of electron density along ZnO n^+-n-n^+ diode under different lattice

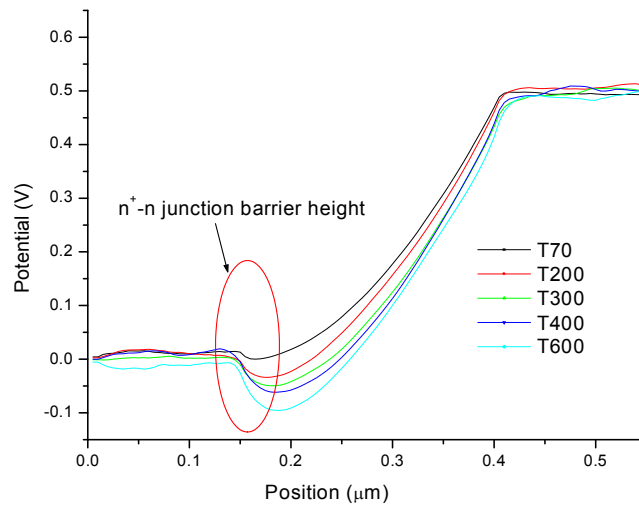


Figure 7. Electrical potential along ZnO n^+-n-n^+ diode under different lattice temperature.

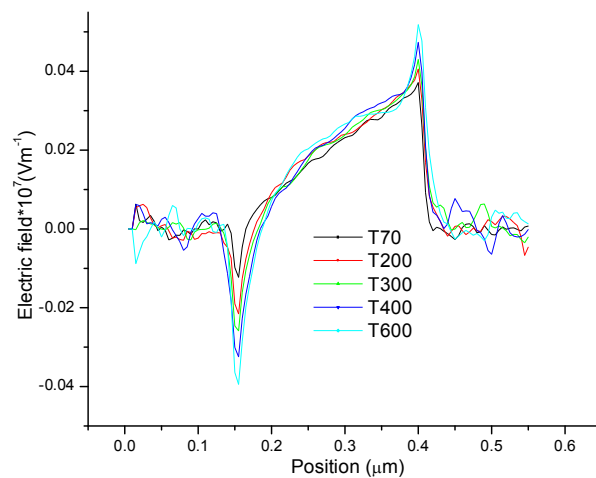


Figure 8. Electric field along ZnO n^+-n-n^+ diode under different lattice temperature.

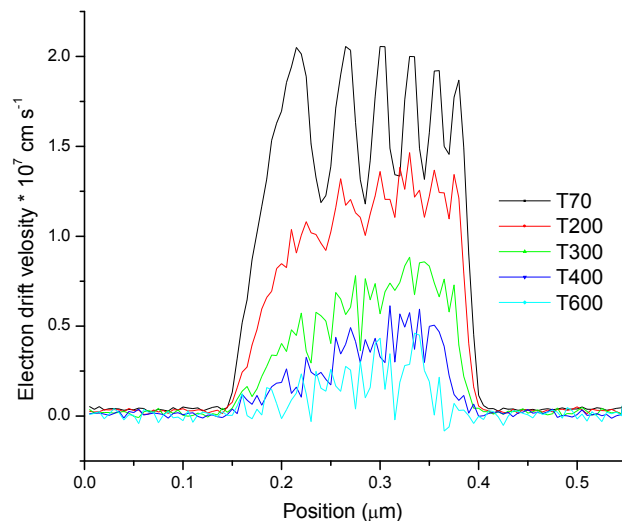


Figure 9. Electron velocity along ZnO n^+-n-n^+ diode under different lattice temperature.

CONCLUSIONS

The results of simulations of electron transport in $n^+-i(n)-n^+$ ZnO diodes has been reported. The diodes have highly doped n^+ -layers serving as the cathode and anode. The anode voltages ranged from 1 to 5 V at room lattice temperature. The electrons injected from the cathode initially travel quasi-ballistically but there is substantial transfer to the upper satellite valleys as the anode is approached, resulting in a reduced average electron velocity in that region. Due to higher velocity-field characteristic it is shown that ZnO based devices should expect to have more performance than SiC or GaN materials.

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