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ORIGINAL ARTICLE

Simulation of High Field Electron Transport in Wurtzite Phase of ZnO

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ABSTRACT
Temperature and doping dependencies of electron drift velocity in wurtzite ZnO structure have been calculated using ensemble Monte Carlo method in steady-state and transient situation. The following scattering mechanisms, i.e, impurity, polar optical phonon and acoustic phonon are included in the calculation. The maximum electron drift velocity that is obtained at room temperature for 10^{23} m^{-3} donor concentration is 2.2×10^{7}cm/s for ZnO. For high applied electric field, transient electron drift velocity shows a significant overshoot.
Keywords-: *Ensemble Monte Carlo, Drift velocity, Overshoot, Steady-state.*

INTRODUCTION

At the start of 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, rspectively) are on the rise and may be regarded as third-generation semiconductors after Si (first-generation with band-gap 1.12 eV) and GaAs and InP (second-generation with band-gap 1.43 and 1.35 eV, respectively). The control of free-carrier concentration is vital for the performance of all semiconductor devices. The intrinsic carrier concentration (n_i) is exponentially dependent on the temperature:

$$n_i = \sqrt{N_C N_V}\, e^{-E_g/2k_BT}$$

Where E_g is the band-gap, k_B is Boltzmann's costant and T is the temperature in Kelvin. It's evident that in high temperatures the WBS have much lower intrinsic carrier concentrations than Si and GaAs. This implies that devices for higher temperatures should be fabricated from WBS to avoid the effects of thermally generated carriers [1]. Also, the WBS are of potential interest as a suitable material high power electronics and because of their direct band gap are benefit for optoelectronic devices, too. ZnO has recently received much attention because of its potential advantages over GaN, including commercial availability of bulk single crystals, amenability to wet chemical etching and a large exciton binding energy (60 meV, compared with 25 meV for GaN) that causes excitonic emission at room and higher temperatures. Although, the exellent radiation hard characteristics, make ZnO a suitable candidate for space applications [2-7]. The present work studies the high-field transport properties for electrons in bulk ZnO in both steady-state and transient situations using ensemble Monte Carlo. It's organized as follows. Details of the simulation model which is used in this work are presented in Sec. II, and results for simulation are interpreted in Sec. III-1 for steady-state and Sec. III-2 for transient situation.

SIMULATION MODEL

In this research for studing of the electron transport within a semiconductor, an ensemble Monte Carlo approach is used in order to solve the Boltzman transport equation (BTE), the BTE describes how the electron distribution fuction evolves under the action of an applied electric field. In this approach, the motion of a large number of electrons within a semiconductor, under the action of an applied electric field, is simulated. The acceleration of each electron in the applied electric field, and the present of the scattering, are both taken into account. The scattering events that an individual electron experiences are selected randomly, the probability of each such event being selected in proportion to the scattering rate corresponding to that particular event. The analysis of electron transport is restricted within the conduction band. Typically, only the lowest part of the conduction

band contain a significant fraction of the electron population instead of including the entire electron band structure for the conduction band, so only the lowest valleys need to be represented and in this work a three valley model is used [8-10].

Within the framework of this three valley model, the nonparabolicity of each valley is treated through the application of the Kane model, the energy band corresponding to each valley being assumed to be spherical and is the form of [9,10]:

$$E(k)[1+\alpha_i E(k)]=\frac{\hbar^2 k^2}{2m^*}$$

where m^* is the electron effective mass in ith valley and α_i is the nonparabolicity coficient in ith valley.

The scattering mechanisms considered are ionized impurity, polar optical phonon, acoustic diformation potential and intervalley scattering. For steady-state and transient electron transport simulations, the motion of eighty thousand electrons are examined in three valleys of Γ, U and K. The material parameters and valley parameters that are used in this simulation are mentioned in table 1.

Table 1. Important parameters used in the simulations for wurtzite phase ZnO [11].

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, $\hbar\omega_{op}$(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

RESULT

1-Steady-state electron transport

Figure 1 shows the velocity-field characteristics that obtained by our model for ZnO wurtzite in 300K temperature and with the 10^{23} m^{-3} donor concentration. It has a peak in its velocity-field characteristic and so show the negative differential mobility. The peak drift velocity is around 2.24×10^7 cm/s in threshold field of 340 kV/cm. As the effective mass of the electrons in the upper valleys is greater than it in the lowest valley, the electron in the upper valleys will be slower. As more electrons transfer to the upper valleys, the electron drift velocity decreases. This leads the negative differential mobility in the velocity field characteristic depicted in Fig. 1[3]. The other important things that is seen in Fig. 1 is dependence of drift velocity on electric field presents a dual-slope behavior before the peak velocity which may be traced back to the onset of polar optical scattering[6]. The valley occupation for the Γ, U and K valleys are shown in Fig. 2. For fields lower than the threshold field, most of the electrons are in the central valley and significant intervalley scattering into the satellite valleys occurs just for fields above the threshold field. The total average electron kinetic energy as a function of electric field is shown in Fig. 3. It can be seen that, kinetic energy increases with the electric field due to the large proportion of electrons in the low mass Γ valley. However, as the field increases the electrons transfer to higher valleys with higher mass and increased scattering which causes a substantial reduction in the rate of increasing of energy. The effect of temperature on steady-state electron drift velocity, valley occupancy and total average energy have been studied and the results are shown in Fig. 4-6. Fig.4 shows that the temperature

increasing causes the drift velocity decreasing. On the other hand the peak velocity occurs in the higher electric fields when the temperature increases. In Fig. 5 you can see the increasing temperature causes the transition of electrons to the satellite valleys starts at higher field with slower rate. Total average electron kinetic energy decreases with increasing temperature as be shown in Fig. 6. We know temperature increasing increases the acoustic phonon scattering and impurity scattering, so electron mobility and drift velocity decreases. On the other hand, it causes electrons loss their energy in scattering events and so transition to satellite valleys decreases.

Fig.7 shows the various doping concentration do not has considerable effect on the drift velocity. Because the scattering of ionized impurity is dominated in low temperatures, so the drift velocity doesn't affect of changing the doping concentration in room temperature.

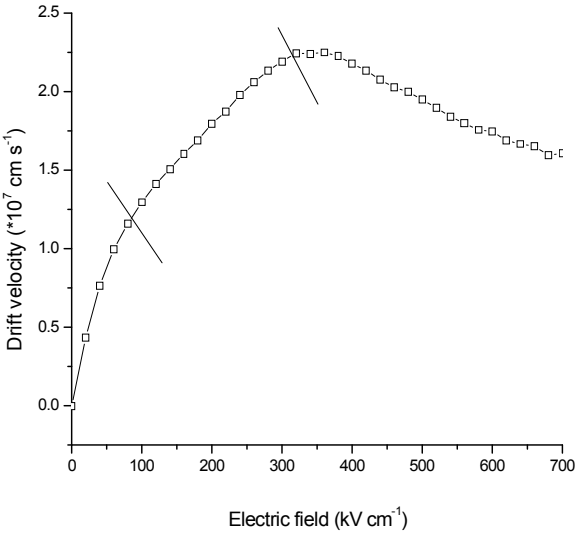

Fig.1. Calculated electron drift velocity in wurtzite ZnO at T=300 K and 10^{23} m^{-3} impurity concentration.

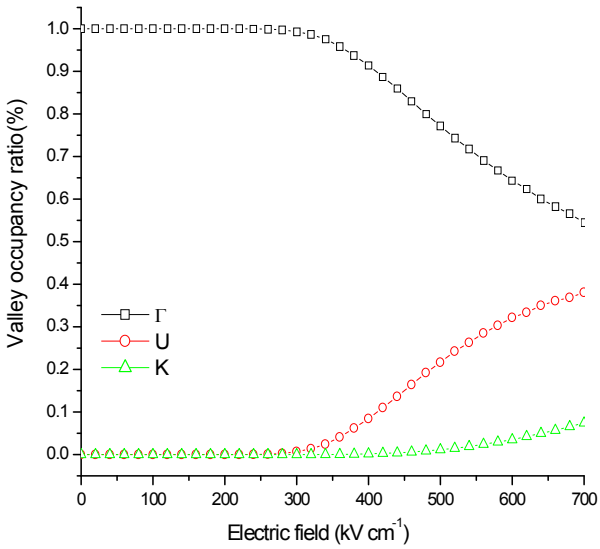

Fig. 2. Calculated valley occupancy ratio in wurtzite ZnO at T=300 K and 10^{23} m^{-3} impurity concentration

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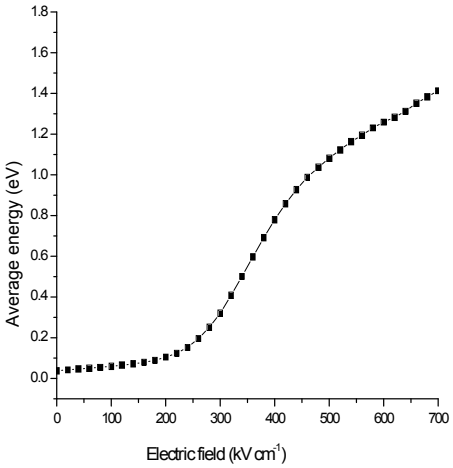

Fig. 3. Total average electron kinetic energy in wurtzite ZnO at T=300 K and 10^{23} m^{-3} impurity concentration.

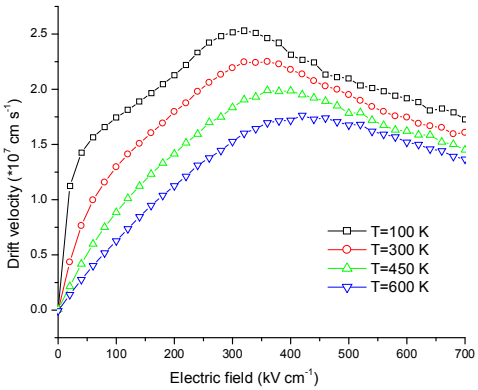

Fig.4. Calculated electron drift velocity in wurtzite ZnO at 10^{23} m^{-3} impurity concentration and different temperatures.

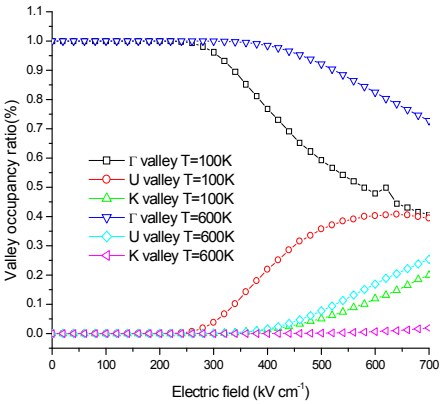

Fig.5 Calculated valley occupancy ratio in wurtzite ZnO at 10^{23} m^{-3} impurity concentration and different temperatures.

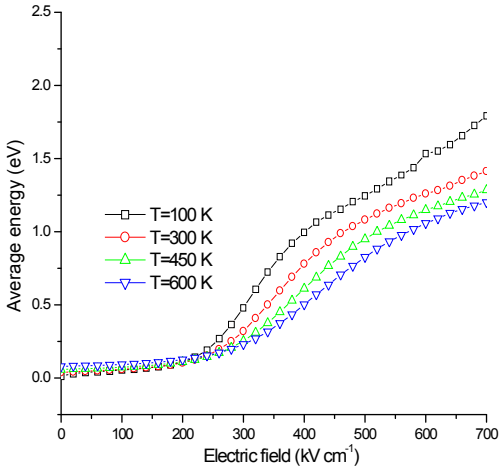

Fig.6. Total average electron kinetic energy at 10^{23} m^{-3} impurity concentration and different temperatures.

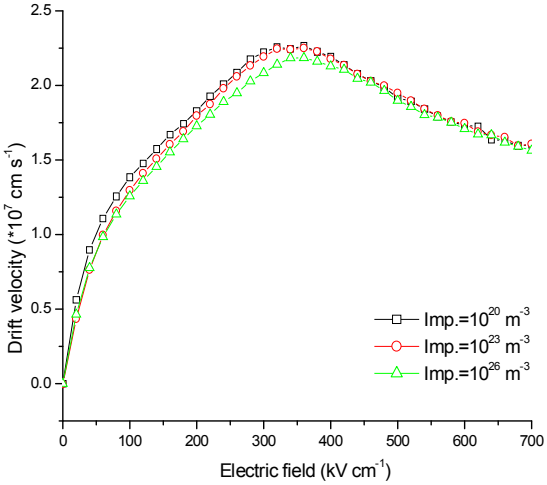

Fig.7. Calculated electron drift velocity in wurtzite ZnO at T=300 K and different impurity oncentrations.

2- Transient electron transport

Fig.8 shows the transient behavior simulated in ZnO. It can be see, for the applied electric field lower than the threshold field electron drift velocity reaches steady-state very quickly with little or no velocity overshoot. In contrast, for applied electric field that is larger than threshold field, transient electron drift velocity shows a significant overshoot. In low electric fields the most of electrons are in central valley with lower effective mass, so the scattering rate is low and transient drift velocity reaches steady-state quickly. But by increasing the applied electric field electrons can gain more energy and by pass the time they could go to the upper valley. In upper valleys, electron effective mass is larger and it causes the scattering rate increases, too. When the scattering rate increases the drift velocity decreases and an overshoot occurs. If applied electric field become more larger, because the electron can gain energy of field sooner the overshoot occurs sooner, too.

Transient behavior dependence on temperature are shown in Fig. 9 for two applied electric field, one of them is lower than threshold field and another is larger than threshold field. It can be seen for constant electric field, when temperature increases like the steady state situation because of increasing scattering rate, drift velocity decreases but the time behavior is independent of temperature. Transient drift velocity versus distance is calculated, too. The result is shown in Fig. 10.

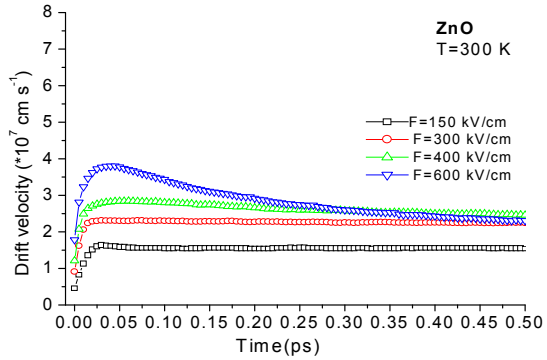

Fig.8. The calculated time evolution of the electron drift velocity at T=300 K for different values of the electric field.

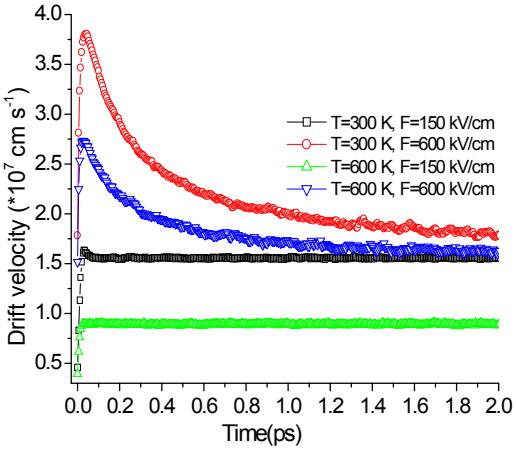

Fig.9. The calculated time evolution of the electron drift velocity in wurtzite ZnO for different values of the electric fields and temperature.

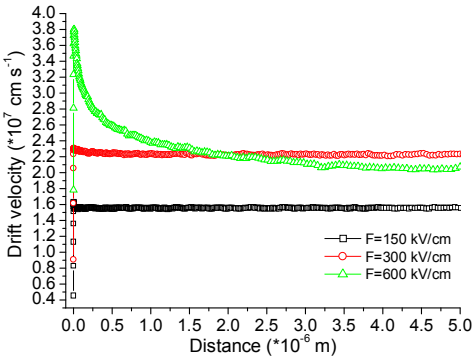

Fig. 10. The calculated distance evolution of the electron drift velocity in wurtzite ZnO at T=300 K.

CONCLUSION

The computed steady-state and transient electron transport in wurtzite ZnO show that, this material has superior electron transport properties. The velocity-field characteristics of the materials show similar trends, reflecting the fact that this semiconductor has satellite valley effective densities of states several times greater than the central gamma-valley. We have also shown that ZnO exhibits much more pronounced overshoot effects compared to other nitride materials but at much higher electric fields. Using valley models to describe the electronic band structure, it is found that electron drift velocity relaxes to the saturation value within 3 ps in ZnO crystal structure.

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