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Electronic Transport Properties in Bulk ZnO and $Zn_{1-x}Mg_xO$ Using Monte Carlo Simulation

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Abstract- In this paper, an investigation with the application of Monte Carlo simulations to steady-state electron transport and low-field electron mobility characteristics of in bulk ZnO in the wurtzite crystal structure and its alloy $Zn_{1-x}Mg_xO$ with different doping of Mg, x=0.05, 0.1 and 0.2. The Monte Carlo calculations are carried out using a three-valley model for the systems under consideration. 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 1.97×10^{7} cms^{-1} for ZnO in threshold field of 400 kV/cm. While the maximum electron drift velocity is 1.62×10^{7} cms^{-1}, 1.03×10^{7} cms^{-1} and 0.43×10^{7} cms^{-1} for $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and $Zn_{0.8}Mg_{0.2}O$ in threshold field 700 kV/cm respectively. It can be seen the peak drift velocity for bulk ZnO is $1.97\times10^{7}cms^{-1}$, while for $Zn_{1\_x}Mg_xO$ the peak drift velocity decreases due to increasing electron effective mass.

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Abstract- In this paper, an investigation with the application of Monte Carlo simulations to steady-state electron transport and low-field electron mobility characteristics of in bulk ZnO in the wurtzite crystal structure and its alloy $Zn_{1-x}Mg_xO$ with different doping of Mg, x=0.05, 0.1 and 0.2. The Monte Carlo calculations are carried out using a three-valley model for the systems under consideration. 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 1.97×10^7 cms^{-1} for ZnO in threshold field of 400 kV/cm. While the maximum electron drift velocity is 1.62×10^7 cms^{-1},1.03×10^7 cms^{-1} and 0.43×10^7 cms^{-1} for $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and $Zn_{0.8}Mg_{0.2}O$ in threshold field 700 kV/cm respectively. It can be seen the peak drift velocity for bulk ZnO is $1.97\times10^7cms^{-1}$, while for $Zn_{1-x}Mg_xO$ the peak drift velocity decreases due to increasing electron effective mass.

We find about valley occupancy in this materials that for fields lower than the threshold field, most of the electrons are in the central valley and significant inter valley scattering into the satellite valleys occurs just for fields above the threshold field.

Finally for electron mobility shows the maximum electron mobility for ZnO is 886 $cm^2/V.s$ and for $Zn_{1-x}Mg_xO$ in various amount x=0.05, 0.1 and 0.2 is 304, 132 and 33 $cm^2/V.s$ respectively. The electron mobility of ZnO is more than ZnMgO alloys at all temperatures because electron mobility behavior dependence on effective mass and ionized impurity concentration.

Keywords: Electron Transport, Monte Carlo Simulation, Wurtzite $Zn_{1-x}Mg_xo$, Effective Mass.

I. Intruduction

Recently, the material properties of ZnO and $Zn_{1-x}Mg_xO$ has attracted much attention [1-8]. This interest has been fuelled, in large measure, by the considerable promise that these materials offer for novel electronic and optoelectronic device. ZnO possesses material properties that makes it particularly suitable for a number of important electronic and optoelectronic device applications. The important properties for ZnO include its wide and direct energy gap of 3.43 (eV), small effective mass, large inter valley energy separation, and large polar optical phonon energy. ZnO is an exhibit favorable electron transport characteristics, so a number of studies of the electron transport that occurs within this material have been reported over the years. Based on these fundamental properties, ZnO has many applications in the short wavelength region, such as optically pumped lasers, UV light emitting diodes, detectors, solar cells, gas sensor and many other advantages, make ZnO a strong candidate for the next generation of ultraviolet light emitting and lasing devices operating at high temperatures and in harsh environments [9-11].These material properties suggest that bulk ZnO will exhibit favorable electron transport characteristics, i.e., elevated steady-state electron drift velocities [12].

Of course it should be pointed out that ZnO is a group transparent conductive oxide (TCO) material. The transparent conductive oxide (TCO) materials, such as ZnO, In_2O_3, Ga_2O_3, Al_2O_3 are fundamental components in optoelectronic devices [6,7]. In 1999-now, Albrecht et al. and Arabshahi et al. reported on Monte Carlo simulations of the steady-state electron transport that occurs within bulk wurtzite ZnO [4,5].

Studies indicate that ZnO with ZnMgO alloys like $Zn_{1-x}Mg_xO$ can improve some properties optoelectronic devices [1-6]. The purpose of the present paper studying the steady-state transport in high electric field and in low filed electron mobility within Bulk ZnO and $Zn_{1-x}Mg_xO$ by three-valley Monte Carlo simulation analysis in 10000 electrons. It is 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 electron mobility.

II. Model Details

In this research for studying 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 function 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

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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. Within the framework of this three valley model, the non parabolicity 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:

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

Where m* is the electron effective mass in it valley and α_i is the non parabolicity coefficient in it valley. The scattering mechanisms considered are ionized impurity, polar optical phonon, and acoustic deformation potential and inter valley scattering. For electron transport properties in Bulk ZnO and $Zn_{1-x}Mg_xO$ Materials simulations, the motion of 10000 electrons is examined in three valleys of Γ, U and K. The material parameters and valley parameters that are used in this simulation are mentioned in tables I and II.

Table 1 : Material parameters for wurtzite ZnO [5]

Parameters	Unit	ZnO
Mass density	kg/m	**5600**
Static relative permittivity	ε_0	**8.2**
High frequency relative permittivity	ε_∞	**3.7**
Polar optical phonon	ev	**0.072**
Piezoelectric constant	C/m^2	**0.089**
Acoustic deformation potential	ev	**14**
Sound velocity	m/s	**6400**
Direct energy gap	ev	**3.43**

Table 2 : Valley parameters for wurtzite ZnO and $Zn_{1-x}Mg_xO$ [5,6]

Valley (ZnO)	Unit	Γ	U	K
Electron effective mass	m^*/m_0	0.318	0.42	**0.7**
Non parabolicity coefficients	1/ev	0.312	0.059	**0.65**
Equivalent valley number	-	1	6	**2**
Valley separation	ev	0	2.1	**2.9**

Valley ($Zn_{1-x}Mg_xO$)	Unit	Γ	U	K
Effective mass for x = 0.05	m^*/m_0	0.462	0.61	**1.015**
Effective mass for x = 0.1	m^*/m_0	0.7338	0.969	**1.61**
Effective mass for x = 0.2	m^*/m_0	1.5586	2.05	**3.4**

III. Results

a) Steady-State Electron Transport

Figure 1 shows the velocity-field characteristics that obtained by our model for ZnO wurtzite and $Zn_{1-x}Mg_xO$ with different doping of Mg, x=0.05, 0.1 and 0.2 in 300K temperature and in the 10^{23} m^{-3} donor concentration. It can be seen, the electron drift velocity increases by high electric field. As soon as the electrons drift velocity and electric field reached to electrons thermal velocity and threshold field, so the electrons are scattered from Γ valley to satellite valleys with more electrons effective mass. In upper valleys the electrons effective mass increase and scattering rate of electrons increase, so the drift velocity decreases. Therefore this scattering creates a peak velocity in curve of drift velocity-electric field. The simulations suggest that the peak drift velocity for bulk ZnO is 1.97×10^7 cm/s in threshold field of 400kV/cm, while the maximum drift velocity for $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and $Zn_{0.8}Mg_{0.2}O$ is 1.62×10^7 cm/s, 1.03×10^7 cm/s and 0.43×10^7cm/s in threshold field of 700 kV/cm respectively. The results shows that the electrons drift velocity decreases in ZnMgO alloys due to have effective mass more than ZnO in satellite valleys, so the scattering rate of electrons increase and mobility and drift velocity of electrons decreases in this valleys. These results of Monte Carlo simulation are in good agreement with the others calculation [6].

Figures 2 shows the calculated electron drift velocity as a function of high electric field at the different temperature. It can be seen 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.

The valley occupation for the Γ, U and K valleys are shown in Figure 3. It is obvious that the inclusion of satellite valleys in the simulation is important. Significant electron transfer to the upper valleys only begins to occur when the field strength is very close to the threshold value. For electric fields lower than the threshold field, most of the electrons are in the central valley and significant inter valley scattering into the satellite valleys occurs in electric fields above the threshold field for ZnO and each of ZnMgO alloys. The reason can be explained in terms of different electron effective masses for this materials within the central valley. This is important because electrons which are near a valley minimum have small kinetic energy and therefore strongly scattered. At the threshold field 400 kv/cm in bulk ZnO for Γ the electron valley occupancies at room temperature is 100%. And in electric field more than threshold field like 500 kV/cm the electron valley occupancies are about 95% in Γ valley and 4% in U valley. Also we know, the effective mass in ZnMgO alloys are more than ZnO, so for the ZnMgO alloys intervalley scattering into the satellite valleys occurin stronger electric fields.

The total average electron kinetic energy as a function of electric field is shown in Figure 4. 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.

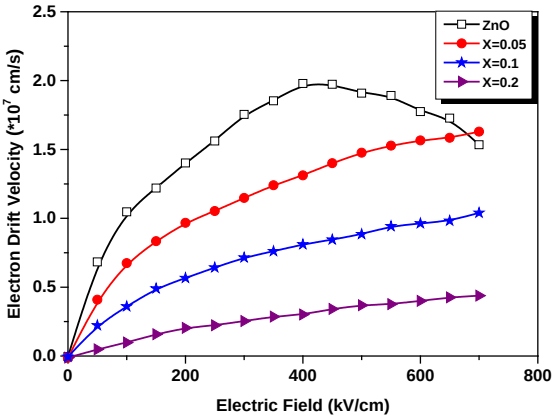


Figure 1 : Calculated electron drift velocity in wurtzite ZnO, $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and $Zn_{0.8}Mg_{0.2}O$ at T=300 K and 10^{23} m^{-3} impurity concentration

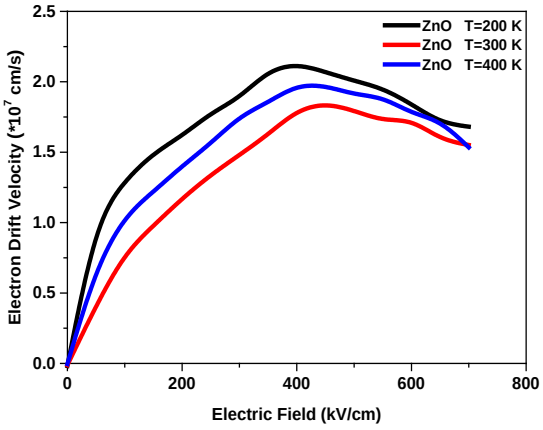


Figure 2 : Calculated electron drift velocity in bulk ZnO at 10^{23} m^{-3} impurity Concentration and different temperatures

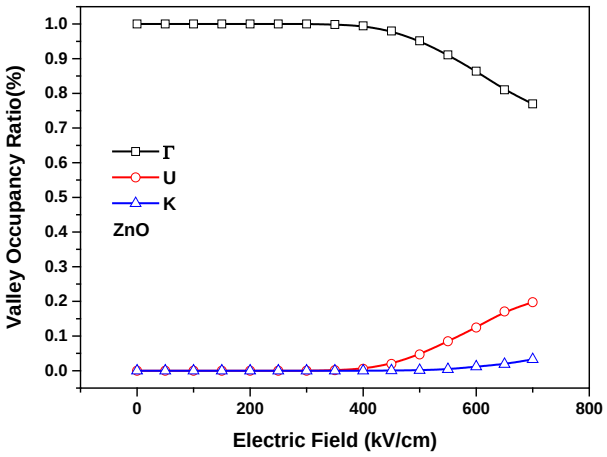


Fig 3 : A

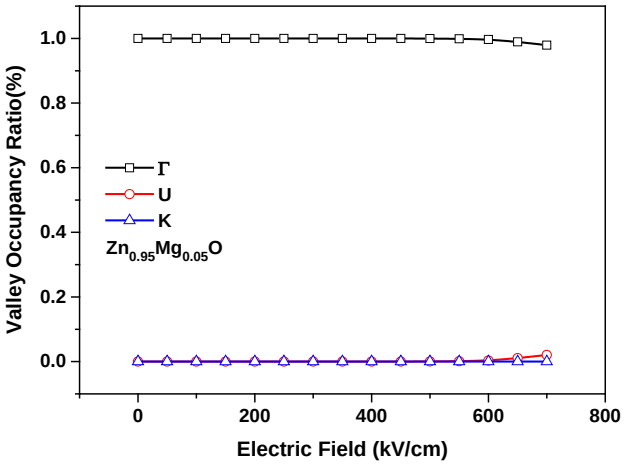


Fig 3 : B

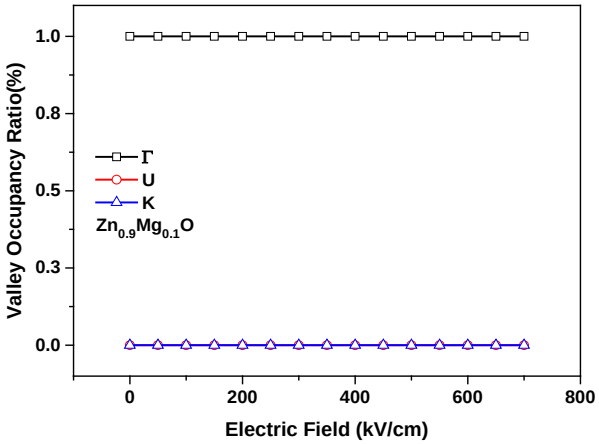


Fig 3 : C

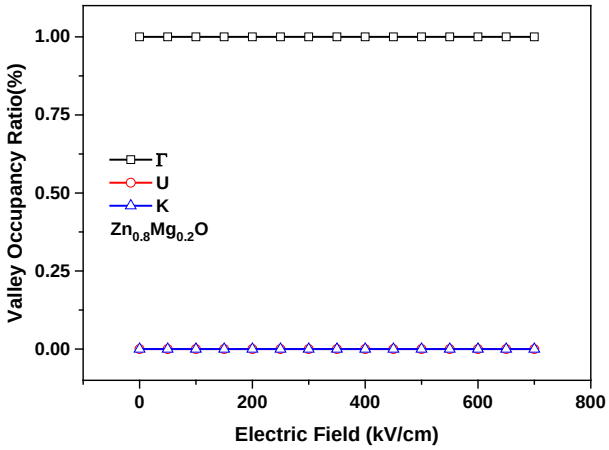
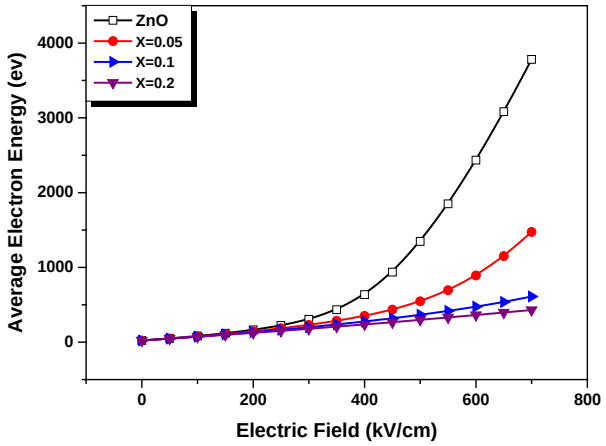


Fig 3 : D

Figures 3 : Calculated valley occupancy ratio in bulk ZnO and ZnMgO alloys at T=300K and 10^{23} m^{-3} impurity concentration



Figures 4 : Total average electron kinetic energy in bulk ZnO and ZnMgO alloys at T=300 K and 10^{23} m^{-3} impurity concentration

b) Electron Mobility

The electron mobility calculates in low field because changing curve drift velocity-electric field is high before threshold field, so the mobility in low field is important. But after threshold field, changing drift velocity in terms of electric field is a little and also the electron mobility decrease. The mobility values are found from each curve of the slope of the linear part of each velocity–field curve.

Figure 5 shows the calculated electron mobility in term temperature in bulk ZnO, $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and $Zn_{0.8}Mg_{0.2}O$ at the 10^{23} m^{-3} impurity concentration. It can be seen that the electron mobility at room temperature for ZnO is 886 $cm^2/V.s$ and for $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and $Zn_{0.8}Mg_{0.2}O$ is 304, 132 and 33 $cm^2/V.s$ respectively. The results indicate that the electron mobility of ZnO is more than ZnMgO alloys at all temperatures. This is largely due to the higher valley effective mass in the ZnO phase. Increasing temperature is increased phonons scattering rate and energy of phonons, so it causes a strong interaction between electrons and these phonons that its result is increase of electrons scattering rate and finally decrease of the electrons mobility. Figure 6 show that the electron mobility decrease by the electrons concentrations increasing because electrons increasing causes increase of ionized impurity centers in crystals that it causes times more electrons under the influence of the coulomb potential of impurity centers located that its result is increase of electrons scattering rate and finally decrease of electrons mobility.

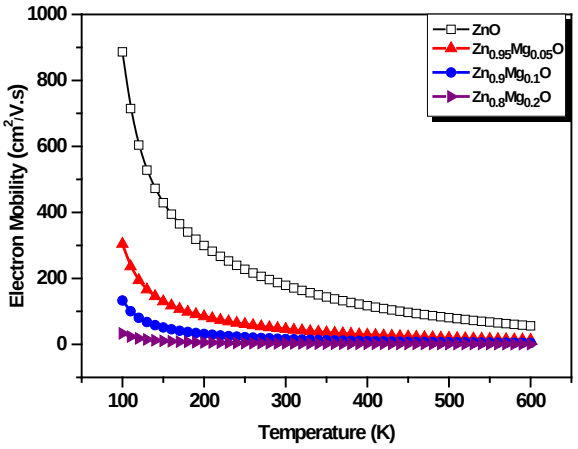


Figure 5 : Changes the electron mobility function in terms of temperature in bulk ZnO and ZnMgO alloys at the10^{23} m^{-3} impurity concentration

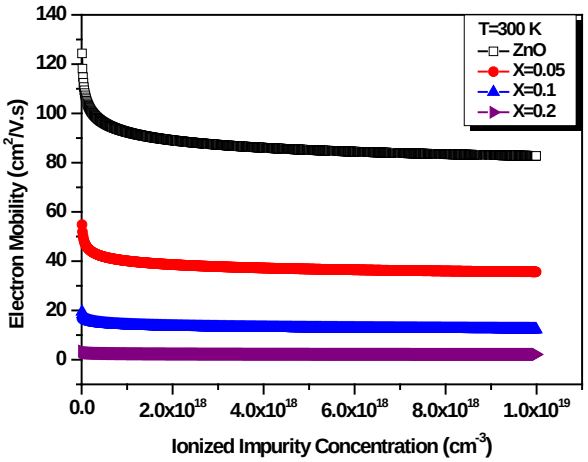


Figure 6 : Changes the electron mobility function in term of ionized impurity concentration in bulk ZnO, $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and $Zn_{0.8}Mg_{0.2}O$ at room temperature

IV. Conclusion

This research presents is about electron transport properties in bulk ZnO and $Zn_{1-x}Mg_xO$ materials performed with ensemble Monte Carlo simulation for different temperatures and ionized impurity concentrations.

These calculations for bulk ZnO and $Zn_{1-x}Mg_xO$ show superior electron transport properties that in this study we obtained some the results for application this materials in device semiconductors:

1. The band gap, drift velocity, mobility and cutoff frequency of bulk ZnO can be controlled by MgO alloys in $Zn_{1-x}Mg_xO$ materials and in this case the electron effective mass increases and the electron mobility decreases. Therefore we can control peak velocity and saturation velocity of threshold field in this materials.
2. The ZnMgO alloys are stronger than ZnO, because the threshold field in ZnMgO alloys is higher than ZnO. Therefore these days in engineering science that use this materials in semiconductors.
3. Comparison of ZnO and ZnMgO alloys show the electrons drift velocity in ZnMgO alloys are less susceptibility to changing temperature. Therefore devices that are made by ZnMgO alloys are more resistant versus high temperature and heat and these devices have more efficiency.
4. The electron mobility in ZnO semiconductor is upper than of ZnMgO alloys because the effective mass in ZnO is lower than $Zn_{1-x}Mg_xO$. Also the ionized impurity scattering in both the semiconductor ZnO, $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and $Zn_{0.8}Mg_{0.2}O$ at all temperatures is an important factor in reducing the mobility.

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