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# Steady-state and transient electron transport in bulk ZnO and $Zn_{1-x}Mg_xO$ semiconductors

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## ABSTRACT

In thiswork, an investigation of the steady-state electron transport and transient electron transport at high electric field and low-field electron mobility characteristics of wurtzite ZnO and $Zn_{1_x}Mg_xO$ are examined using the ensemble Monte Carlo model. 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 concentrations is $2.36\times10^7$ $cms^{-1}$ for ZnO in threshold field 461 kV/cm. While the maximum electron drifts velocity is $1.65\times10^7$ $cms^{-1}$ for $Zn_{0.95}Mg_{0.05}O$ in threshold field 861 kV/cm. The maximum electron mobility for ZnO886 $cm^2$/V.s and for $Zn_{1_x}Mg_xO$ in variuos amount x=0.05, 0.1 and 0.2 is 304, 132 and 33 $cm^2$/V.s respectively. It can be seen the peak drift velocity for bulk ZnO is $2.36\times10^7$ $cms^{-1}$, while for $Zn_{1_x}Mg_xO$ the peak drift velocity decreases due to increasing electron effective mass. The electron mobility of Zno is more than ZnMgo alloysat all temperatures becauseelectron mobility behavior dependence on effective mass and ionized impurity concentration.
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## KEYWORDS

Electron Transport;
Monte Carlo simulation;
Wurtzite $Zn_{1_x}Mg_xO$,
Effective mass.

## INTRODUCTION

Recently, the material properties of ZnO and $Zn_{1-x}Mg_xO$ have attracted much attention[4-10]. 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 3.37 (eV), small effective mass, large inter valley energy separation, and large polar optical phonon energy. ZnO is an exhibit favorable electron transport characteristic 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[1-12]. In 1999, Albrecht et al. reported on Monte Carlo simulations of

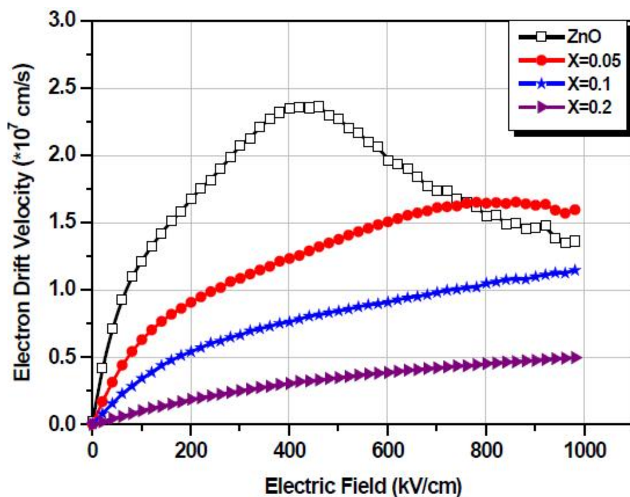


**Figure 1: Calculated electron steady-state drift velocity in bulk ZnO, $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and$Zn_{0.8}Mg_{0.2}O$ at T=300 K and $10^{23}$ $m^{-3}$ impurity concentration**

the steady-state electron transport that occurs within bulk wurtzite ZnO was that reported by Arabshahi et al.[4-6]. Studies indicate that ZnO with ZnMgO alloys like $Zn_{1-x}Mg_xO$can improve some properties optoelectronic devices[7]. The purpose of the present paper is to calculate electron drift velocity and electron mobility in bulk ZnO and $Zn_{1-x}Mg_xO$ for different Mg contents for a wide range of temperature and ionizedimpurity concentrations by three-valley Monte Carlo simulation analysis in ten thousand electrons. It is organized as follows. Details of the simulation model which is used in this work are presented insection II, and the results for simulation are interpreted in section III.

## MODEL DETAILS

The ensemble Monte Carlo techniques have been used for well over 30 years as a numerical method to simulate non equilibrium transport in semiconductor materials and devices and has been the subject of numerous books and reviews. The Monte Carlo method as applied to semiconductor transport is a simulation of the trajectories of individual Carriers as they move through a device under the influence of external forces and subject to random scattering events. The duration of the carrier free flights between successive collisions and the scattering events involved are selected stochastically in accordance with the given transition probabilities describing the microscopic processes. Two of the great advantages of semi classical Monte Carlo are its capability to provide accurate quantum mechanical treatment of various distinct scattering mechanisms within the scattering terms, and the absence of assumption about the form of carrier distribution in energy or k-space. In our model, the conduction band is approximated by non-parabolic multi valley bands, using the dispersion relation.

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

where m* is the electron effective mass in the valley and ±i is the non-parabolic coefficient in the valley.

The scattering mechanisms considered are ionized impurity, polar optical phonon, acoustic deformation potential and inter valley scattering. In this simulations, the motion of ten thousand electrons are examined in three valleys.

## RESULTS

### Steady-state electron transport

Figure1 shows drift velocity-electric field characteristics in bulk ZnO and $Zn_{1_x}Mg_xO$ for various Mg content at 300 K temperature and withthe $10^{23}$ $m^{-3}$ donor concentration. It can be seen, the electron drift velocity increasedbyhigh 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 higher energy andelectrons effective mass increases, so electronsmobility 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 around $2.36\times10^7$ $cms^{-1}$in threshold field 461 kV/cm. While for $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and $Zn_{0.8}Mg_{0.2}O$ is $1.65\times10^7$, $1.14\times10^7$ and $0.49\times10^7cms^{-1}$respectively. The threshold field for $Zn_{1_x}Mg_xO$is (x=0.05) 861 kV/cm, (x=0.1) 981 kV/cm and (x=0.2) 981 kV/cm. The results shows that the electrons drift velocity decreases in $Zn_{1_x}Mg_xO$due to have effective mass more than ZnO in satellite valleys, so the electron drift velocity decreases. These results of Monte Carlo simulation havea good agreement with the others calculation[7].

Figures 2 show the calculated electron drift velocity as a function of high electric field at the dif-

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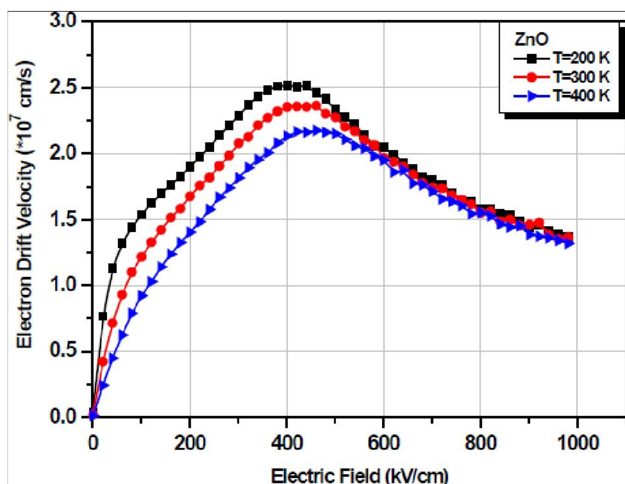


**Figure 2: Calculated electron steady-statedrift velocity in bulk ZnO at the different temperature and $10^{23}$ $m^{-3}$ impurity concentration**

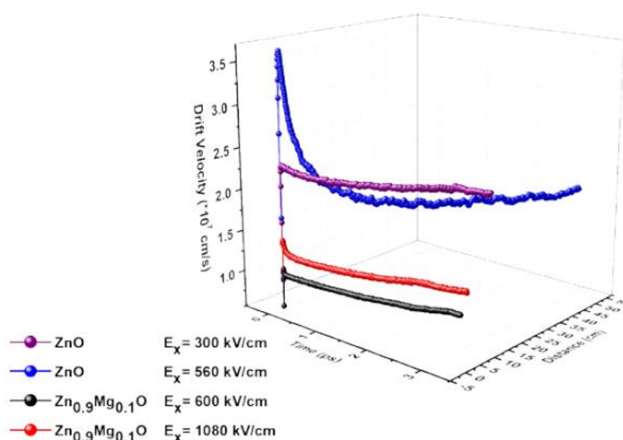


**Figure 3: A comparison of the velocity overshoot effect exhibited in ZnO and $Zn_{0.9}Mg_{0.1}O$ as calculated by Monte Carlo simulation at room temperature**

ferent temperature. The decrease of drift velocity with temperature in electric field lower than threshold field is due to the increase intra valley scattering (scattering of acoustic phonons, piezoelectric and ionize impurity). Also it shows that the peak drift velocity decreases by increasing temperature in high electric field. This is due to that total scattering rate is increasing with high temperature and total electrons energy decreased, so the electrons population in the Γ valley are increased and in satellite valleys decreases.

## Transient electron transport

Transient electron transport is the changes drift velocity in term of time for different applied electric fields. So that in electric field lower than threshold filed the electron drift velocity reaches steady-state very quickly with little or no velocity overshoot and the electrons are in central valley. By increasing electric field more than threshold filed the overshoot occurs and the electrons can go to satellite valleys. Because the electrons gain more energy and by pass the time they could go to the upper valley.

We examined transient electron transport in bulk ZnO and $Zn_{0.9}Mg_{0.1}O$. The transient responses of electrons in these materials are compared in Figure 3 to 5 for different electric fields and temperature. (In this section Figures Drift velocity are plotted in 3D in term Time and Distance). The threshold filed is 461 kV/cm for ZnO and 981 kV/cm for $Zn_{0.9}Mg_{0.1}O$. We calculated transient transport in two electric field like 300 and 560 kV/cm for ZnO and for $Zn_{0.9}Mg_{0.1}O$ in electric fields 600 and 1080 kV/cm.

Figure 3 shows the transient behavior for ZnO and $Zn_{0.9}Mg_{0.1}O$. In this study is observed 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 compare, for applied electric field that is larger than threshold field, transient electron drift velocity shows a substantially overshoot. We note that in low electric fields the most of electrons are in central valley with lower effective mass, so the scattering rate is a little and transient drift velocity reaches to steady-state very 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 also 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 earlier the overshoot occurs earlier. The transient behavior dependence on temperature is also studied in Figures 4 and 5 for two applied electric field in two materials. one of electric fields is lower than threshold field and another is upper than threshold field. In this figure shows, for constant electric field when the temperature increases in the steady state position the peak of velocity decreased and increasing scattering rate, but the time behavior is independent of temperature. Also transient drift velocity versus distance is calculated.

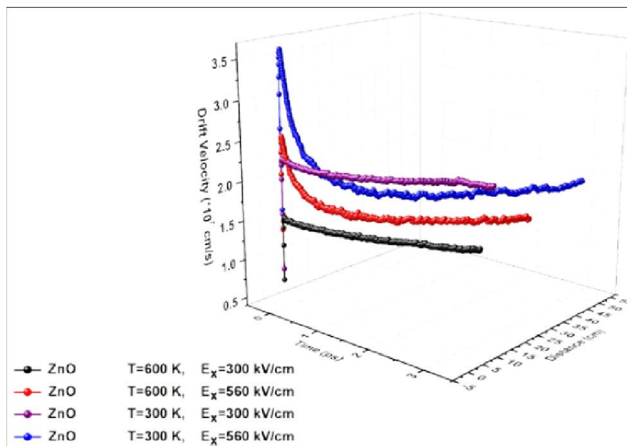


**Figure 4: The velocity overshoot effect exhibited in ZnO as calculated by Monte Carlo simulation at different temperature**

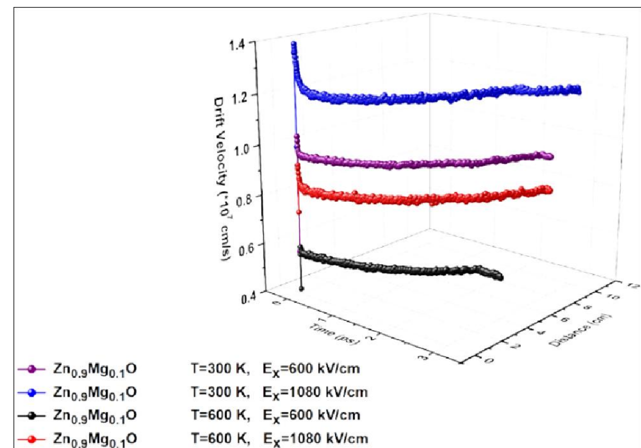


**Figure 5: The velocity overshoot effect exhibited in ZnO and $Zn_{0.9}Mg_{0.1}O$ as calculated by Monte Carlo simulation at different temperature**

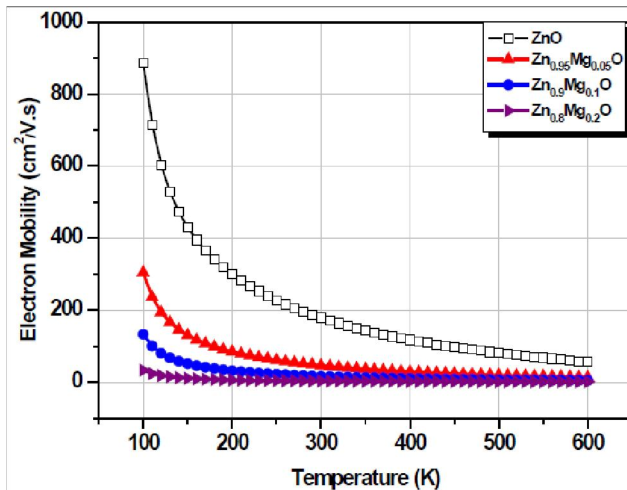


**Figure 6: Changes the electron mobility function in terms of temperature in bulk ZnO and$Zn_{1_x}Mg_xO$at the $10^{23}$ $m^{-3}$ impurity concentration**

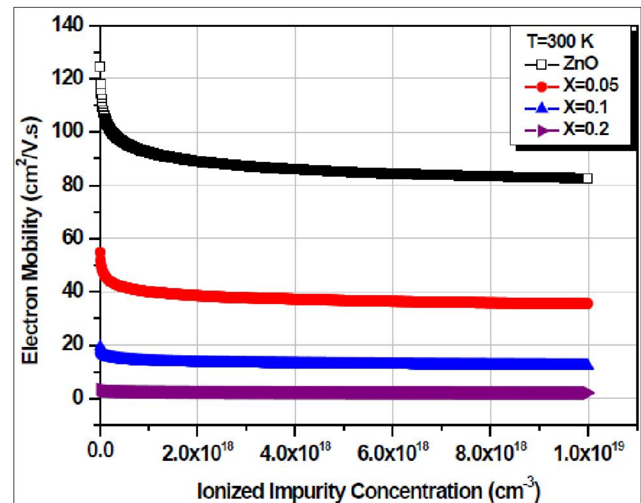


**Figure 7: Changestheelectron mobility as a function of ionizedimpurity concentration in bulk ZnO, $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and $Zn_{0.8}Mg_{0.2}O$ at room temperature**

The result is shown in Figures 3 to 5.

## Electron mobility

The electron mobility calculates in low field because changing curve drift velocity-electric field is highbefore 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; therefore the electron mobility is very low. Satellite valleys do not affect the low-field mobility calculation since no inter valley transfer occurs at low electric field inconsequently, the low-field mobility is attributed solely to transport of Γvalley electrons.

Figure 6 shows the calculated electron mobility in term temeraturein 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 seenthat the electron mobilities at roomtemperature 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 $Zn_{0.8}Mg_{0.2}O$is304, 132 and 33 $cm^2$/V.s respectively. The results indicatethat the electron mobility of Zno is more than ZnMgo alloysat all temperatures. This is largely due to the higher valley effective mass in the ZnO phase. Increasing temperture 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 7 show that The electron mobility decrease by the electrons concentrations increasing because electrons increasing causes increase of ion-

ized 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.

## CONCLUSION

In this paper we can be seen, the velocity–field curves in bulk ZnO exhibit overshoot peaks for electric fields of approximately 461 kV/cm. The same overshoot effect is observed in ZnO with various Mg contents. While the peak velocity decreases as the Mg content increases, the field at which the peak velocity is attained increases. Also, we examined transient electron transport in this materials. It can be seen transient behavior depended on effective mass, applied electric field strength, temperature and distance. The low-field electron mobility values are extracted from the slope of the linear part of each velocity–field curveand then we showed the electron mobility behavior dependence on effective mass and ionized impurity concentration. The ionized impurity scattering in ZnO and$Zn_{1_x}Mg_xO$at all temperatures is an important factor in reducing the mobility.

The ZnMgO alloys are stronger than ZnO, because the threshold field in ZnMgO alloys is higher than ZnO. Therefore today's in engineering science used of these materials in semiconductors. Comparison of ZnO and $Zn_{1_x}Mg_xO$show the electrons drift velocity in $Zn_{1_x}Mg_xO$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.

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