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Assessment of Monte Carlo Simulation of Electron Transport in ZnO Diode in Intelligent Information Systems

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Abstract: Aim: The interest to study electron transport in semiconductor devices at very high electric field has been increased in the last decades and assessment of Monte Carlo simulation of electron transport in ZnO diode in intelligent information systems is of high significance. Method: 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. Monte Carlo simulation is performed to study quasi-ballistic transport of electrons in n^+nn^+ ZnO diode. Result: In this simulation, the spatial motion of the electrons is semi classical and the scattering mechanisms taken into account are those due to acoustic phonons, non-polar optical phonons, polar optical phonons and ionized impurities. The simulation results are reported for different temperatures and voltages. Conclusion: It is also found that the transient properties of ZnO-made diode are not much sensitive to environment temperature changes, and thus the use of this substance is highly recommended in manufacture of electronic equipment.

Keywords: Ensemble Monte Carlo, Ellipsoidal Valleys, Brillouin Zone, Drift Velocity

1. Introduction

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 [1]. 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 [2]. 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 [3-5].

Nowadays, most components in the electronics industry are made in sub-micrometer dimensions. Therefore, the properties of electron transport in these particles are very different from those of a semiconductor volume or of parts with dimensions larger than micrometer, due to the intense and non-uniform electric field produced along these parts. Thus todays, extensive research is conducted on sub-micrometer electronic components such as n^+nn^+ diodes known as ballistic diodes [6]. Various methods are available to study the transport properties of the carriers in electronic components, where one of the most important methods for understanding the physical properties is the Monte Carlo method [7].

Recently, the material properties of ZnO and Zn1-xMgxO have attracted much attention. 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 [F2]. 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 [8-10].

In current study, the results of the Monte Carlo simulation of electron transport properties is studied in a sub-micrometer n^+nn^+ ZnO diode, at various temperatures and voltages. The considered semiconductor in this simulation is ZnO, where this substance has a Wurtzite structure and a direct band gap of 3.4 electron volts. The important parameters of the material used in this research are given in Table 1 [11].

Table 1. *Parameters of ZnO substance.*

Parameter	Size	Parameter	Size
$\rho(kg/m^3)$	5675	$\hbar\omega_0(ev)$	0.073
$\varepsilon_s\ (F\ /\ m)$	8.2 ε_0	$\Xi_d(ev)$	15
$\varepsilon_\infty\ (F\ /\ m)$	3.7 ε_0	$D_{ii}(ev/\ m)$	1×10^{11}
$v_s\ (m\ /\ s)$	6590	$E_g(ev)$	3.4

2. Simulation Method

Monte Carlo simulations are used to model the probability of different outcomes in a process that cannot easily be predicted due to the intervention of random variables. It is a technique used to understand the impact of risk and uncertainty in prediction and forecasting models. Monte Carlo simulation can be used to tackle a range of problems in virtually every field such as finance, engineering, supply chain, and science. Monte Carlo simulation is also referred to as multiple probability simulation.

Monte Carlo simulation performs risk analysis by building models of possible results by substituting a range of values—a probability distribution—for any factor that has inherent uncertainty. It then calculates results over and over, each time using a different set of random values from the probability functions. Depending upon the number of uncertainties and the ranges specified for them, a Monte Carlo simulation could involve thousands or tens of thousands of recalculations before it is complete. Monte Carlo simulation produces distributions of possible outcome values. By using probability distributions, variables can have different probabilities of different outcomes occurring. Probability distributions are a much more realistic way of describing uncertainty in variables of a risk analysis.

Using the Monte Carlo ensemble method, the transport characterizes the electrons in the n^+nn^+ ZnO diode has been investigated in sub-micrometer dimensions. In this simulation, the effects of non-stationary state of energy strips are considered, and the number of examined particles is from the order of 10^5 size. In this semi-classical method, carriers are considered as classical particles, which are influenced by various dispersion processes. The dispersion mechanisms considered in this simulation are due to the acoustic phonon dispersion, polar optical phonon, ionized impurities, and the dispersion of non-polar optical phonons. [12-15]. The elastic dispersion of ionized impurities is also considered by the Coulomb Potential of Brooks- Herring type [16-18].

The structure of the n^+nn^+ diode used in this simulation is shown in Figure 1. As seen from the figure, the middle region (N CHANNEL) is placed between the two anode and cathode regions, with concentration of higher impurities, and various voltage differences of 1.5, 3 and 4.5 Volts are applied to the both ends of component to examine the transport properties.

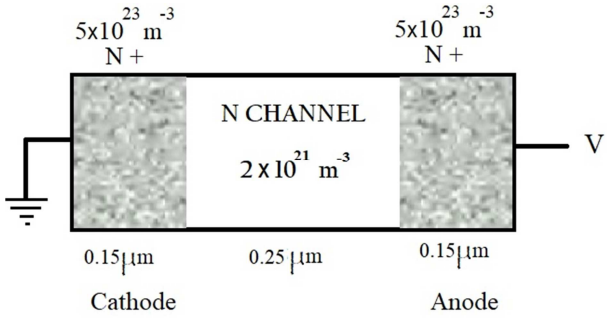

Figure 1. *n^+nn^+ diode Structure.*

3. Simulation Results

In Figure 2, the electric field diagram is plotted against the length of the ZnO diode for 1.5, 3 and 4.5 volts. As seen in this figure, the electric field is emitted from the cathode to the anode. This field is published in such a way that, as the orbit closes closer to the anode region, the electric field increases sharply and with the voltage increase the created field in middle zone of diode increases drastically as well.

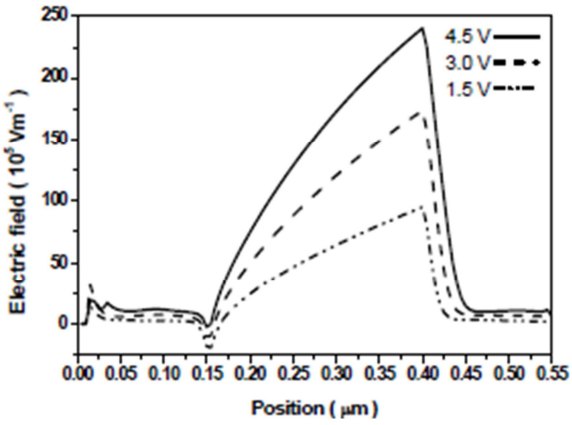

Figure 2. *Diagram of electric field against the ZnO diode length at room temperature for 1.5, 3 and 4.5 volts.*

In Figure. 3, the density diagram of electrons is plotted against the length of diode for 1.5, 3 and 4.5 volts. The electron density in two cathode and anode regions is equal to the density of contaminated impurities in these two regions. The electrons are dispersed from the anode and cathode to the middle layer, and electrons are accelerated to the anode region through an electric field produced in the middle region. According to the figure, with increasing voltage the density of scattered electrons increases toward the middle region.

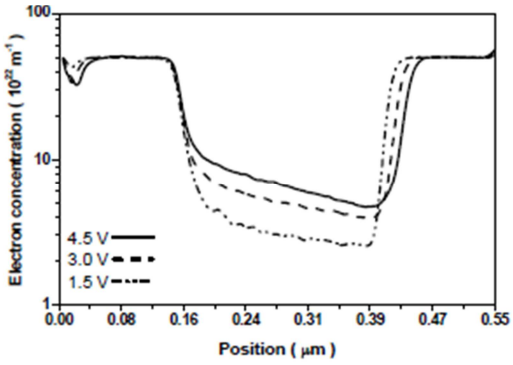

Figure 3. *Electron Density Characteristic against the ZnO diode length at room temperature for 1.5, 3 and 4.5 volts.*

Figure 4 refers to changes in velocity of electrons in relation to the length of component for applied voltages of 1.5, 3 and 4.5 volts at room temperature. As seen in the figure, the speed of propulsion increases with increasing applied voltage. As the voltage increases, stronger electric fields are produced in the middle region, which increases the average energy of the carriers, and as a result, the electrons move faster, and the amount of electron interaction decreases with the covered Coulomb potential, and leads to reduction in dispersion rate and increment in speed of the carrier.

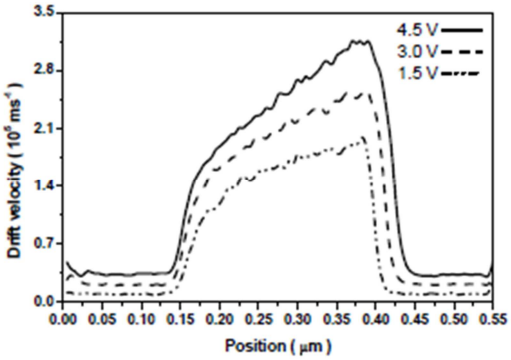

Figure 4. *The velocity curve of electrons against the length of ZnO diode at room temperature for voltages of 1.5, 3 and 4.5 volts.*

In Figure 5, velocity variations of electrons along the ZnO segment for 3 volts at 150, 300, 450 Kelvin are plotted. Given the fact that the dispersion rate is directly related to temperature, with increasing temperature, the dispersion rate rises, and as a result, the speed of carrier decreases.

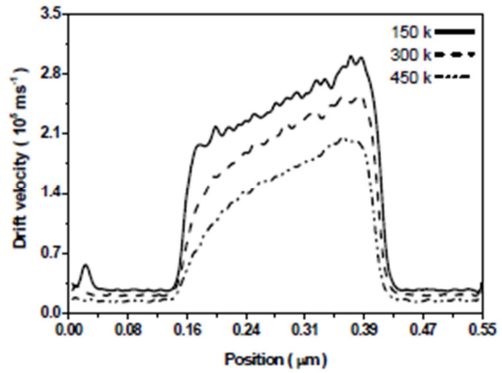

Figure 5. *The velocity curve of electrons against the length of ZnO diode for voltage of 3 V at 150, 300, 450 K.*

In Figure 6, the kinetic energy curve shows the average electrons along the segment for a voltage of 3 volts and for temperatures of 150, 300, 450 Kelvin. As seen from the figure, at temperatures of 300 Kelvin, electrons reach an average energy of the order of 0.14 in the near-Andean region. At this energy level, due to the large bandwidth of ZnO material, the carriers transmitted energy They will not have higher energy valleys. Due to the presence of electrons in the central valley, the average energy of the electrons increases due to the increase in the temperature.

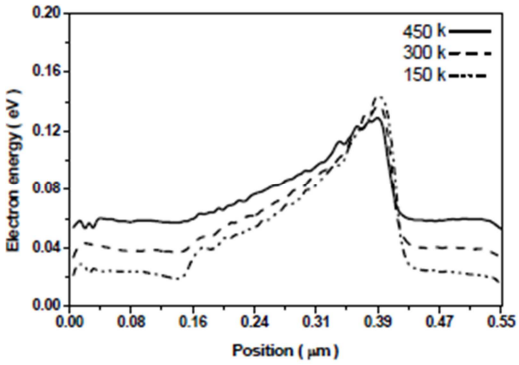

Figure 6. *Graph of average kinetic energy of electrons against the ZnO diode length for applied voltage of 3 V at 150, 300, 450 K.*

The potential graph along the segment length resulted of Poisson equation's solution is presented Figure 7, in the time interval of 2 x 10^{-12}s for ZnO diode at 150, 300, 450 Kelvin. As shown in the figure, the applied voltage in the two cathode and anode regions is a constant value, and is 0 and 3 volts, respectively. Where it continuously changes between these two values throughout the mid-zone of potential. The reason for these changes can be interpreted according to Figure 3. Given the fact that the density of electrons in the two cathode and anode regions is equal to the density of impurities that are contaminated in these two regions, while the density of net charge of carriers *(n (x) - N_d (x))* is zero through these two regions, then according to equation (1) (Poisson equation) the potential will have a constant value in these two regions according to equation (2).

$$\nabla^2\phi = -{}^{e}/_{\varepsilon_0}\,(n(x) - N_d(x)) \qquad (1)$$

$$\nabla^2\phi = 0 \;\rightarrow\; \phi = Const. \qquad (2)$$

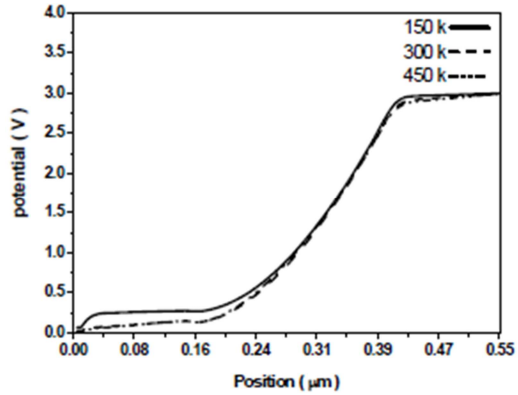

Figure 7. *Potential diagram against the ZnO diode length for applied voltage of 3V at 150,300,450 K.*

The results of Monte Carlo method and the results of other methods for simulating the electron transport properties in semiconductor components are in very good agreement when compared with experimental results [6].

4. Conclusion

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. The Monte Carlo ensemble simulation results indicate that the ZnO ballistic diode in the form of n^+nn^+ has a high efficiency in production of electronic components. And this is due to the strong increase in voltage of the electric field in middle region of diode, which increases the speed of electrons.

It is also found that the transient properties of ZnO-made diode are not much sensitive to environment temperature changes, and thus the use of this substance is highly recommended in manufacture of electronic equipment.

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