Monte Carlo simulation of electron mobility in a material for optoelectronics at 77 K

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The electron mobility values have been obtained at 77K using the Monte Carlo simulation technique. The values agree satisfactorily with available data. The mobility values thus obtained have then been expressed by simple power law relationship. It is observed that the mobility values calculated by using these simple power law relations yield values that show agreement within 5% with those obtained from the detailed Monte Carlo simulation technique. We conclude that such empirical relationships can be effectively used for quick determination of mobility values at different electric fields in a device-modelling program and in the development of CAD tools.

(Received February 11, 2010; accepted April 11, 2010)

Keywords: Zinc oxide**,** Monte Carlo simulation, Electron mobility, Empirical relation

1. Introduction

Recently, ZnO is being considered as one of the most suitable materials for optoelectronic applications like blue/Ultra Violet light sources and detectors, solar blind UV photodetectors and transparent field effect transistors, etc., [1]. ZnO is not new as a material, the mechanical, chemical, electrical, and optical properties of ZnO and other technological issues such as growth, defects, *p*-type doping, band-gap engineering, nanostructures have already reported by many authors long back [2], but recently it has received renewed attention mainly because of its potential advantages over nitrides, commercial availability of bulk single crystals, amenability to wet chemical etching, a larger exciton binding energy, and excellent radiation hardness [2, 3].

Though it is already mentioned that many properties of ZnO are well studied, not much work have been done yet on transport properties of this II-VI compound semiconductor. Recently, Baozeng Guo *et al* have obtained mobility values of electron at room temperature, 200K and 500K[4]. With all these in mind, we have presented in this paper, the velocity-field characteristics of ZnO at 77K using the Monte Carlo (MC) simulation technique. The mobility values thus obtained have then been expressed by the simple power law relationships, the coefficients of which are determined by least mean square fit (LMSF) technique. It is found that the mobility values obtained from such simple power law relationships agree quite satisfactorily with the results obtained from detailed MC simulation and also with the available experimental data.

To obtain the carrier transport properties, one has to solve the Boltzmann transport equation (BTE) taking the various scattering mechanisms for the charge carriers into account. Scattering by optical phonons, which are of the polar type in II-VI compound semiconductors, is known to be predominant in these materials [5-6] and a solution of the Boltzmann equation with predominant polar optical phonon scattering is beset with many complications, particularly under a large applied electric field when high energetic optical phonons dissipate the energy of the electron system to the lattice in an inelastic fashion. To obviate these difficulties, one has to take recourse to numerical techniques like the Monte Carlo simulation technique which has now become an important tool for device simulation. In this technique, the motion of the electron through the semiconductor is simulated in a digital computer by using random numbers and taking into account the probabilistic nature of the various electron-lattice collision processes. The motion of a single electron is followed through a large number of collisions, and the principle of ergodicity is invoked to obtain the ensemble average from the time average of a single particle.

2. Scattering rate calculation

The free flight of a carrier through the lattice is disturbed by collisions with lattice vibrations and impurity atoms. Let, at an instant of time t, the wave vector of the carrier be **k**. If the carrier suffers a collision at time t its wave vector changes from **k** to **k**$^{/}$.

The scatterings that have been considered here are scattering by ionized impurity atoms, by polar optical phonons and by acoustic phonons through deformation potential coupling and through piezoelectric interaction.

Each of these collisions is characterized by the scattering rate S_i (**k**) which is the number of collisions of the ith type per unit time per unit volume in the **k** space.

$$S_i(k) = V_c \Big/ \left(4\pi^2\hbar\right) \int \left|M(k,k')\right|^2 \delta\,(E_K - E_{K'})\,dk' \qquad (1)$$

where V_c is the crystal volume. M_i (k, k$^{/}$) = is the matrix element for ith scattering mechanism for scattering from k state to k$^{/}$ state, and may be written as

$$\left|M_i\left(k,k'\right)\right|^2 = \left[A_i\left(\left|k - k'\right|\right)\right]^2 G\left(k,k'\right)$$

G(k, k′) is the overlap function, and A_i is the matrix element without the overlap function and is given [7], for the different scattering mechanisms as

$$A_{imp} = \left(Z e^2 / V_c \varepsilon\right)\left(\left|k - k'\right|^2 + \lambda^{-2}\right)^{-1}$$

$$A_{ac} = E_1\left(\hbar / 2 V_c \rho \omega_q\right)^{1/2}\left(e_q . q\right) F\left(q,\lambda\right)$$

$$A_{pz} = \left(e h_{pz} / \varepsilon\right)\left(\hbar / 2 V_c \rho \omega_q\right)^{1/2} F\left(q,\lambda\right)$$

$$A_{pop} = \left(e/q\right)\left(\kappa_\infty^{-1} - \kappa_0^{-1}\right)\left(\hbar\omega_l / 2 V_c \varepsilon_0\right)^{1/2} F(q,\lambda)$$

where

$$F\left(q,\lambda\right) = S_c\left(q,\lambda\right)\left(n_q + \tfrac{1}{2} \pm \tfrac{1}{2}\right),$$

λ is the Debye screening length, E_1 is the acoustic phonon deformation potential coupling constant, e_q is the unit lattice vector, h_{pz} is the piezoelectric constant, ω_l is the longitudinal polar optical phonon frequency, $q = |k - k'|$, Z is the degree of ionization of the impurity atoms, assumed unity and screening factor is given by

$$S_c\left(q,\lambda\right) = q^2 / \left(q^2 + \lambda^{-2}\right)$$

Substituting the appropriate matrix elements and carrying out the integration in (1), the scattering rates were evaluated for the different scattering processes.

It is to be noted that in Monte Carlo calculations, the polar optical phonon emission and absorption are treated as two separate processes. It is found, that the total scattering rate decreases rapidly with energy up to the optical phonon energy when optical phonon emission takes place and the total scattering rate increases at this energy. The total scattering rate then decreases as all the scattering rates except that for acoustic phonons are, in general, decreasing functions of energy. Above an energy of about 3eV the total scattering rate, however, increases with energy due to increasing occurrence of acoustic phonon scattering. In an actual simulation a maximum energy value is chosen such that the electron energy almost never reaches that high value and the Rees' parameter, Γ is taken as the total scattering rate at that chosen maximum energy. This choice obviously requires an a-priori knowledge of this variation of the total scattering rate with energy in the material. The type of variation of the total scattering rate as described above is characteristic of the II-VI compound semiconductors and is the same for all the semiconductors considered here.

3. The Monte Carlo simulation procedure

The carrier is presumed to start with an initial wave vector k_o. Under the influence of the external electric field, it accelerates and continues its motion in what is called its free flight. The duration of the free flight is estimated by a pseudorandom number r_o distributed uniformly between 0 and 1. The time at which the collision takes place is given by

$$t_c = -\left(\ln r_0\right)/\Gamma \tag{2}$$

where Γ is the chosen Rees' parameter. Γ has been rendered constant over the energy range considered by including a self-scattering term such that the sum of all the real scattering rates plus the self-scattering rate remains constant over the entire energy range considered. It has been shown that the steady state value obtained by including the self-scattering term is indeed the value corresponding to the real scatterings [8]. The wave vector of the carrier at the end of the free flight is k and this is computed by using the laws of classical mechanics. Once t_c is determined, one may obtain the trajectory of the electron from 0 to t_c by using the laws of Newtonian mechanics.

Having determined the instant at which the free flight has been terminated, one has to determine the type of collision that terminated the free flight. The scattering rates S_i corresponding to the various scattering mechanisms for the carrier with wave vector **k** are then computed by using the expressions detailed in [7]. Next, another random number r_1 is used to ascertain which one of the n scattering mechanisms including the self scattering processes has been operative. The j^{th} mechanism is chosen to terminate the free flight, if

$$\left(\sum_{i=1}^{j} S_i \Big/ \sum_{i=1}^{n} S_i\right) \le r_1 < \left(\sum_{i=1}^{j+1} S_i \Big/ \sum_{i=1}^{n} S_i\right) \tag{3}$$

Having determined the kind of scattering, the energy and the wave vector of the electron after a real collision are determined from the conservation of the energy and the momentum. The energy of the electron after collision is given by E + ΔE, where ΔE is the change in energy induced by the collision and E is the energy of the electron immediately before the collision. It is given by

$$E = \hbar^2 k^2 \left(t_c / 2 m^*\right)$$

For acoustic, piezoelectric and ionized impurity scatterings ΔE is taken equal to zero while for polar optical phonon scattering it is equal to $\pm \hbar \omega_l$.

The magnitude of the electron wave vector after the collision is then given by

$$k_i = \left[2 m^* \left(E + \Delta E\right)\right]^{1/2} / \hbar$$

This value of the wave vector is taken as the initial wave vector for the next free flight.

The orientation of the wave vector after collision is obtained by generating two more random numbers r_2 and r_3, distributed uniformly between 0 and 1. We note that the probability that the polar angle θ and the azimuthal angle φ of the wave vector k_i with respect to any convenient

direction, will be contained in the intervals dθ and dϕ is proportional to Sinθdθdϕ. θ and ϕ can, therefore, be chosen with the random numbers r_2 and r_3 as

$$\cos\theta = 1 - 2r_2$$
$$\phi = 2\pi . r_3$$

The distribution function of the electrons has also been obtained from the results of these computations. For this purpose the entire k space is subdivided into a large number of cells and the time the electron spends in a particular cell of the k space is logged and this value is normalized by the total time. This gives the probability of the electron being in that cell, and hence the energy distribution function. The normalized distribution function thus obtained is shown Fig. 1 for ZnO at 77K for applied electric fields of 5 and 10 kV/cm for zero ionized impurity concentration.

The average velocity can be obtained from displacement and time by dividing the total displacement along the field direction by the total time.

$$v_z = \left(\hbar / m^*\right)\sum_i \left(k_{zo} t_{ci} + \left(eE/\hbar\right)\left(t_{ci}^2/2\right)\right) \Big/ \sum_i t_{ci}$$

The average velocity can also be obtained from the energy and momentum by using the relation [2].

$$v_d = \hbar^{-1} \sum \left(E_f - E_i\right) \Big/ \sum \left(k_{fz} - k_{iz}\right) \qquad (4)$$

where E_i and E_f are respectively the energy after a collision and before the next collision. k_{iz} and k_{fz} are the corresponding components of the wave vector in the field direction. It is to be noted that the velocity values obtained by using the above two methods agree exactly with each other. It may be noted that calculation of velocity by this method is not possible at low fields as the unbalanced part of the random velocities could be comparable to the drift velocity. To avoid this difficulty, the low field mobility is evaluated in the Monte Carlo simulation indirectly through the diffusion constant by using the Einstein relation.

4. Empirical relations

The electron mobility has been calculated in ZnO at 77K for electric fields up to 50 KV/cm by the MC simulation technique. The empirical relations at 77K between electron mobility μ and the applied electric field E is of the form

$$\mu / \mu_0 = 1 + a_1 E + a_2 E^2 + a_3 E^3 \qquad (5)$$

where μ_0 is the low field mobility and the values of the coefficients a_1, a_2, a_3 as well as the calculated values of the low field mobility, μ_0 for ZnO at 77K is shown in Table 1.

Table 1. Values of coefficients for least-mean-squares fit of mobility.

Material	μ_0 ($cm^2v^{-1}s^{-1}$)	a_1 $(kV/cm)^{-1}$	a_2 $(kV/cm)^{-2}$	a_3 $(kV/cm)^{-3}$
ZnO	1867	-5.5E-2	1.6E-3	-1.5E-5

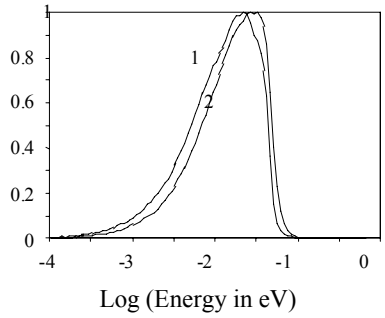

Fig. 1. The normalized distribution function for ZnO at 77K for applied electric fields of 5 and 10 kV/cm for zero ionized impurity concentration. (1) 5 kV/cm (2 10 kV/cm.

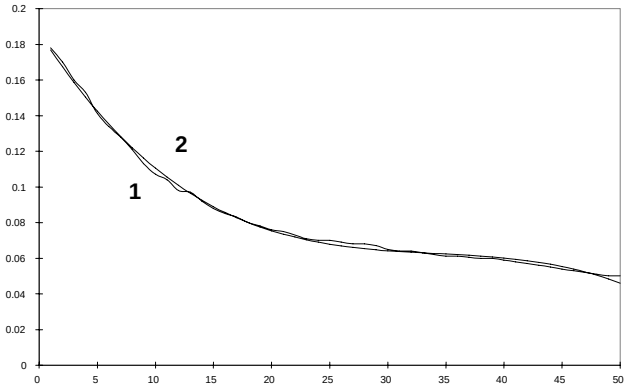

Fig. 2. Variation of electron mobility in ZnO with applied electric field at 77K, (1) Monte Carlo simulation, (2) Empirical Relation [5].

5. Results and discussion

The model for Monte Carlo simulation described earlier is implemented in C. Formulations for computation of different band properties, such as overlap integral, δγ/δE etc. are included in the program. Also included are scattering rate computation routines for various scattering processes. The simulation is found to converge after between 50 and 100 thousand real scatterings depending upon the applied electric field and the material considered.

In Fig. 2, we have plotted the variation of the electron mobility with the applied electric field for ZnO for an ionized impurity concentration of 10^{15} cm^{-3}. It is found that the mobility decreases monotonically with the applied electric field. We have compared the mobility values with the values obtained by empirical relations and shown the comparison in the same figure. We found that by retaining terms up to the 3rd order, the empirical relations give values accurate to within 3% of the values obtained from

the detailed MC simulation technique. The Monte Carlo Simulation results agree with the other available theoretical results. Mukhopadhyay and Bhattacharya theoretically investigated the velocity-field characteristics of ZnO using the displaced Maxwellian model for the energy distribution of the free carriers and considering the combined effects of acoustic, piezoelectric, ionized impurity and polar optical modes of scattering at 77K and 300K [9]. Our present results of ZnO using the Monte Carlo simulation technique agree satisfactorily with those calculations at 77K.

6. Conclusions

It is concluded that the relation (5) between the mobility and electric field will be useful for quick estimation of mobility in II-VI compound semiconductors under high field conditions without having recourse to detailed Monte Carlo technique in device simulation and for quick comparison of experimental data with theoretical results.

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