Influence of Electron-Plasmon Scattering on Low-Field Mobility in ZnO

H. Arabshahi * and M. Rezaee Rokn-Abadi
Physics Department, Ferdowsi University of Mashhad, Mashhad, Iran

Temperature and doping dependencies of electron mobility in ZnO semiconductor has been calculated using an iterative technique. The following scattering mechanisms, i.e., impurity, polar optical phonon, acoustic phonon, piezoelectric, and electron-plasmon are included in the calculation. It is shown that electron-plasmon scattering influence substantially the low-field electron mobility in bulk ZnO. We found that the electron mobility decreases monotonically as the temperature increases from 100K to 600K. The low temperature value of the electron mobility increases significantly as the doping concentration is increased. The iterative results are in fair agreement with other recent calculations obtained using the relaxation-time approximation and experimental methods.

1. Introduction

ZnO is a wide band gap semiconductor, and therefore, has a high breakdown field and low thermal generation rate. These properties combined with good thermal conductivity and stability make ZnO an attractive material for high power, high temperature and radiation harsh environment electronic devices. Monte Carlo simulations predict a peak electron velocity of 3×10^5 ms^{-1} and a saturation electron velocity of 1.3×10^{-5} ms^{-1} [1-5]. This makes possible high frequency operation of ZnO devices. For the above stated reasons, ZnO is of great interest for power FETs and optoelectronic device structures. ZnO based field-effect transistors have been reported to exhibit continuous wave outputs up to 6.9 W/mm [6] and high frequency operation [7] at $f_T = 67$ GHz and $f_{max}=140$ GHz.

The low-field electron mobility is one of the most important parameters that determine the performance of a field-effect transistor. The purpose of the present paper is to calculate electron mobility for various temperatures and ionized-impurity concentrations. The formulation itself applies only to the central Γ valley conduction band. We have also considered band non-parabolicity, admixture of p-type valence-band wave functions, degeneracy of the electron distribution to any arbitrary degree, and the screening effects of free carriers on the scattering probabilities. All the relevant scattering mechanisms, including the two-mode nature of the polar optic phonon and electron-plasmon scattering are taken into account. The Boltzmann equation is solved iteratively for our purpose, jointly incorporating the effects of all the scattering

* arabshahi@um.ac.ir

mechanisms. Our calculated results are compared with the available experimental data on both temperature and the free electron concentration dependence of mobility.

This paper is organized as follows. Details of the iterative model, the electron scattering mechanism, which have been used and the electron mobility calculations, are presented in Sec. 2 and the result of iterative calculations carried out on ZnO structure are interpreted in Sec. 3.

2. Model details

To calculate the mobility, we have to solve the Boltzmann equation to get the modified probability distribution function under the action of a steady electric field. Here, we have adopted the iterative technique for solving the Boltzmann transport equation. Under the action of a steady field, the Boltzmann equation for the distribution function can be written as:

$$\frac{\partial f}{\partial t} + v.\nabla_r f + \frac{eF}{\hbar}.\nabla_k f = \left(\frac{\partial f}{\partial t} \right)_{coll} \qquad (1)$$

Where, $\left(\dfrac{\partial f}{\partial t} \right)_{coll}$ represent the change of distribution function due to electron scattering. In the steady-state and under application of a uniform electric field the Boltzmann equation can be written as

$$\frac{eF}{\hbar}.\nabla_k f = \left(\frac{\partial f}{\partial t} \right)_{coll} \qquad (2)$$

Consider electrons in an isotropic, non-parabolic conduction band whose equilibrium Fermi distribution function is $f_0(\mathbf{k})$ in the absence of

electric field. Note the equilibrium distribution $f_0(\mathbf{k})$ is isotropic in $\mathbf{k}$ space, but is perturbed when an electric field is applied. If the electric field is small, we can treat the change from the equilibrium distribution function as a perturbation, which is first order in the electric field. The distribution in the presence of a sufficiently small field can be written quite generally as

$$f(k) = f_0(k) + f_1(k)\cos\theta \qquad (3)$$

Where, θ is the angle between $\mathbf{k}$ and $\mathbf{F}$ and $f_1(\mathbf{k})$ is an isotropic function of $\mathbf{k}$ proportional to the magnitude of the electric field. $f(\mathbf{k})$ satisfies the Boltzmann equation (Eqn. 2) and it follows that

$$\frac{eF}{\hbar}\frac{\partial f_0}{\partial t} = \sum_i \left\{ \int \cos\varphi f_1^{'} \left[s_i^{'}(1-f_0) + s_i f_0 \right] d^3k^{'} - f_1 \int \left[s_i(1-f_0^{'}) + s_i^{'} f_0^{'} \right] d^3k^{'} \right\} \qquad (4)$$

In general there will be both elastic and inelastic scattering processes. For example, impurity scattering is elastic and acoustic and piezoelectric scattering are elastic to a good approximation at room temperature. However, polar and non-polar optical phonon scattering are inelastic. Labeling the elastic and inelastic scattering rates with subscripts *el* and *inel* , respectively, and recognizing that for any process i, $s_{eli}(\mathbf{k}', \mathbf{k}) = s_{eli}(\mathbf{k}, \mathbf{k}')$, Eqn. 4 can be written as

$$f_1(k) = \frac{\dfrac{-eF}{\hbar}\dfrac{\partial f_0}{\partial k} + \sum \int f_1^{'}\cos\varphi [s_{inel}^{'}(1-f_0) + s_{inel}f_0)]d^3k^{'}}{\sum \int (1-\cos\varphi)s_{el}d^3k^{'} + \sum \int [s_{inel}(1-f_0^{'}) + s_{inel}^{'}f_0^{'}]d^3k^{'}} \qquad (5)$$

Note the first term in the denominator is simply the momentum relaxation rate for elastic scattering.

Eqn. 5 may be solved iteratively by the relation

$$f_{1n}(k) = \frac{\dfrac{-eF}{\hbar}\dfrac{\partial f_0}{\partial k} + \sum \int f_1(k^{'})[n-1]\cos\varphi [s_{inel}^{'}(1-f_0) + s_{inel}f_0)]d^3k^{'}}{\sum \int (1-\cos\varphi)s_{el}d^3k^{'} + \sum \int [s_{inel}(1-f_0^{'}) + s_{inel}^{'}f_0^{'}]d^3k^{'}} \qquad (6)$$

Where, $f_{1n}(k)$ is the perturbation to the distribution function after the *n*-th iteration. It is interesting to note that if the initial distribution is chosen to be the equilibrium distribution for which $f_1(k)$ is equal to zero, then, we get the relaxation time approximation result after the first iteration. We have found that convergence can normally be achieved after only a few iterations for small electric fields. Once $f_1(k)$ has been evaluated to the required accuracy, it is possible to calculate quantities such as the drift mobility, μ, which is given in terms of spherical coordinates by

$$\mu = \frac{\hbar}{3m^*F}\frac{\int_0^\infty (k^3/1+2\alpha F)f_1 d^3k}{\int_0^\infty k^2 f_0 d^3k} \qquad (7)$$

Here, we have calculated low field drift mobility in ZnO structure using the iterative technique. In the following sections electron-phonon, electron-impurity, and electron-plasmon scattering mechanisms will be discussed.

A. Deformation potential scattering

The acoustic modes modulate the inter-atomic spacing. Consequently, the position of the conduction and valence band edges and the energy band gap will vary with position because of the sensitivity of the band structure to the lattice spacing. The energy change of a band edge due to this mechanism is defined by a deformation potential and the resultant scattering of carriers is called deformation potential scattering. The energy range involved in the case of scattering by acoustic phonons is from zero to $2\hbar vk$, where *v* is the velocity of sound, since momentum conservation restricts the change of phonon wave vector to between zero and 2k, where k is the electron wave vector. Typically, the average value of k is of the order of 10^7 cm^{-1} and the velocity of sound in the medium is of the order of 10^5 cms^{-1}. Hence, $2\hbar vk$ ~ 1 meV, which is small as compared to the thermal energy at room temperature. Therefore, the deformation potential scattering by acoustic modes can be considered as an elastic process except at very low temperature. The deformation potential scattering rate with either phonon emission or

absorption for an electron of energy E in a non-parabolic band is given by Fermi's golden rule as [8-9]

$$R_{de}(k) = \frac{\sqrt{2}D_{ac}^2(m_t^{*2}m_l^*)^{1/2}K_BT}{\pi\rho^2\hbar^4} \cdot$$
$$\frac{\sqrt{E(1+\alpha E)}}{(1+2\alpha E)}\left[(1+\alpha E)^2 + 1/3(\alpha E)^2\right] \quad (8)$$

Where, D_{ac} is the acoustic deformation potential, ρ is the material density and α is the non-parabolicity coefficient. The formula clearly shows that the acoustic scattering increases with temperature.

B. Piezoelectric scattering

The second type of electron scattering by acoustic modes occurs when the displacements of the atoms create an electric field through the piezoelectric effect. This can occur in the compound semiconductors such as the III-V and II-VI materials including ZnO that in fact has a relatively large piezoelectric constant. The piezoelectric scattering rate for an electron of energy E in an isotropic, parabolic band has been discussed by Ridley [10], who included the modification of the Coulomb potential due to free carrier screening. The screened Coulomb potential is written as

$$V(r) = \frac{e^2}{4\pi\varepsilon_0\varepsilon_s}\frac{\exp(-q_0 r)}{r} \quad (9)$$

Where, ε_s is the relative dielectric constant of the material and q_0 is the inverse screening length, which under non-degenerate conditions is given by

$$q_0^2 = \frac{ne^2}{\varepsilon_0\varepsilon_s K_B T} \quad (10)$$

Where, n is the electron density. The expression for the scattering rate of an electron in a non-parabolic band structure, retaining only the important terms, can be written as [8-9]

$$R_{pz}(k) = \frac{\sqrt{m^*}e^2 K_{av}^2 K_B T}{4\sqrt{2}\pi\hbar^2\varepsilon_0\varepsilon_s}\gamma^{-1/2}(E)(1+2\alpha E)^2 \times$$
$$\left[\ln(1+\frac{8m^*\gamma(E)}{\hbar^2 q_0^2}) - \frac{1}{1+\hbar^2 q_0^2/8m^*\gamma(E)} + \left(\frac{\sqrt{2}\alpha E}{1+2\alpha E}\right)^2\right]$$
$$(11)$$

Where, K_{av} is the so called dimensionless average electromechanical coupling constant.

C. Polar optical phonon scattering

The dipolar electric field arising from the opposite displacement of the negatively and positively charged atoms provides a coupling between the electrons and the lattice which results in electron scattering. This type of scattering is called polar optical phonon scattering and at room temperature and is generally the most important scattering mechanism for electrons in III-V semiconductors. This is also the case in ZnO despite the fact that the optical phonon energy is particularly high at ~ 93 meV, which suppresses the phonon population and also electrons must reach that energy before phonon emission is possible. The scattering rate due to this process for an electron of energy E in an isotropic, non-parabolic band is [8-9]

$$R_{po}(k) = \frac{\sqrt{2m^*}e^2\omega_{op}}{8\pi\varepsilon_0\hbar}(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_s})\frac{1+2\alpha E'}{\gamma^{1/2}(E)} \times$$
$$F_0(E,E')\{N_{op}, N_{op}+1\} \quad (12)$$

Where,

$$F_0(E,E') = C^{-1}\left\{A\ln\left|\frac{\gamma(E)^{1/2}+\gamma(E')^{1/2}}{\gamma(E)^{1/2}-\gamma(E')^{1/2}}\right| + B\right\}$$
$$A = \left[2(1+\alpha E)(1+\alpha E') + \alpha(\gamma+\gamma')\right]^2$$
$$B = -2\alpha\gamma^{1/2}\gamma'^{1/2}\left[4(1+\alpha E)(1+\alpha E') + \alpha(\gamma+\gamma')\right]$$
$$C = 4(1+\alpha E)(1+\alpha E')(1+2\alpha E)(1+2\alpha E')$$

Where, N_{op} is the phonon occupation number and the upper and lower cases refer to absorption and emission, respectively. For small electric fields, the phonon population will be very close to equilibrium so that the average number of phonons is given by the Bose-Einstein distribution

$$N_{op} = \frac{1}{\exp(\frac{\hbar\omega_{op}}{K_B T})-1} \quad (13)$$

Where, $\hbar\omega_{op}$ is the polar optical phonon energy.

D. Non-polar optical phonon scattering

Non-polar optical phonon scattering is similar to deformation potential scattering. In that, the deformation of the lattice produces a perturbing potential, but in this case the deformation is carried by optical vibrations. The non-polar optical phonon scattering rate in non-parabolic bands is given by [8-9]

$$R_{npo}(k) = \frac{D_{od}^2 (m_t^{*2} m_l^*)^{1/2}}{\sqrt{2}\pi\hbar^3 \rho\omega_{op}} (1+2\alpha E)\gamma^{1/2}(E)[N_{op}, N_{op}+1]$$

(14a)

Where, D_{od} is the optical deformation potential and, $E = E' \pm \hbar\omega_{op}$ is the final state energy phonon absorption (upper case) and emission (lower case).

E. Impurity scattering

This scattering process arises as a result of the presence of impurities in a semiconductor. The substitution of an impurity atom on a lattice site will perturb the periodic crystal potential and result in scattering of an electron. Since the mass of the impurity greatly exceeds that of an electron and the impurity is bonded to neighboring atoms, this scattering is very close to being elastic. Ionized impurity scattering is dominant at low temperatures because, as the thermal velocity of the electrons decreases, the effect of long-range Coulomb interactions on their motion is increased. The electron scattering by ionized impurity centres has been discussed by Brooks-Herring [11], who included the modification of the Coulomb potential due to free carrier screening. The scattering rate for an isotropic, non-parabolic band structure is given by [8-9]

$$R_{im}(k) = \frac{8\pi n_i e^4}{k_s^2 \hbar q_0} (m_t^{*2} m_l^*)^{1/2} \gamma^{1/2}(E) \frac{1+2\alpha E}{1+4\sqrt{2\gamma(E)}(m_t^{*2}m_l^*)^{1/6}/\hbar q_0}$$

(14b)

Where, n_i is the impurity concentration, q_0 is the screening length and k_s is the dielectric constant of the material.

F. Electron-plasmon scattering

The electron-plasmon interaction Hamiltonian can be written in random phase approximation as [12-13]

$$H_{int} = \sum M_q (a_q c_{k+q}^+ c_k + a_{-q}^+ c_{k+q}^+ c_k)$$

(15)

Here, a_q^+, a_q and c_k^+, c_k are the creation and annihilation operators for plasmons and electrons, respectively. The matrix element

$$M_q = \sqrt{\frac{e^2 \hbar^3}{8\Omega \varepsilon m^{*2} \omega_p(q)}} \cdot (2qk+q^2)/q$$

(16)

Where, $\omega_p(q)$ is the dispersion relation for plasmons, q and k are the plasmon and electron momenta, respectively, e and m* are the charge and effective mass of an electron, ε the background dielectric constant, and Ω the real-space volume. The first term in parentheses in Eqn. 15 describes the plasmon absorption process that obeys the energy conservation law as

$$\varepsilon_{k+q} - \varepsilon_k = \hbar\omega_p(q) \geq 0$$

(17)

Where, ε_k is the energy of electron with momentum k. In a similar manner, the plasmon emission process, in accordance with the second term in parentheses in Eqn. 15, is governed by the energy conservation law which can be written as

$$\varepsilon_k - \varepsilon_{k+q} = \hbar\omega_p(q) \geq 0$$

(18)

Note that Eqn. 17 describes the emission of plasmon with momentum -q. To impart a more conventional form to the energy conservation law, replace the variable of summation q in terms governing the plasmon emission in eqn. 1 by -q. Then we can rewrite Eqn. 15 as

$$H_{int} = \sum (M_q a_q c_{k+q}^+ c_k + M_{-q} a_q^+ c_{k-q}^+ c_k)$$

(19)

The notation of Eqn. 15 leads to the following form of the energy conservation law for the emission processes

$$\varepsilon_k - \varepsilon_{k-q} = \hbar\omega_p(q) \geq 0$$

(20)

From the Fermi Golden rule, we can calculate the electron-plasmon scattering rates for emission W_e and absorption W_a

$$W_{e,a}(k) = \frac{2\pi}{\hbar} \int \frac{\Omega dq}{8\pi^3} \left|\langle f|H_{int}|i\rangle\right|^2 \times$$

$$\delta[\varepsilon_{k'} - \varepsilon_k \pm \hbar\omega_p(q)]$$

(21)

Where, k and k' are electron momenta in an initial state $|i\rangle$ and a final state $|f\rangle$, respectively. Here and further, the upper signs in formulae correspond to the plasmon emission, whereas the lower ones do to the plasmon absorption. By using Eqn. 15 and the energy conservation requirements in the forms of Eqns. 18 and 20, which are consistent with this notation of H_{int}, Eqn. 21 becomes

$$W_{e,a}(k) = \frac{2\pi}{\hbar} \int \frac{\Omega dq}{8\pi^3} M_{\mp q}^2 \delta\big[\varepsilon_{k\mp q} - \varepsilon_k \pm \hbar\omega_p(q)\big] \times \atop \{(N_q+1)_{em}; (N_q)_{ab}\} \quad (22)$$

Where, N_q is the Bose-Einstein distribution function for plasmons. The integration bounds with respect to q are defined from the following conditions

$$\omega_p(q) \le \hbar kq / m^* \mp \hbar q^2 / 2m^*$$
$$\omega_p(q) \ge \hbar k_f q / m^* + \hbar q^2 / 2m^* \quad (23)$$

Where, k_f is the electron momentum at the Fermi surface.

3. Results

The electron-plasmon scattering is included only in the low effective mass Γ valley. So, we have just taken into account the temperature and electron concentration dependence of the electron mobility in the Γ valley, which arises due to the different scattering mechanisms. The effect of the electron-plasmon scattering on the electron mobility as a function of temperature is shown in Fig. 1. As it is seen, the inclusion of the electron-plasmon scattering leads to the effective heating of the hot-electron system.
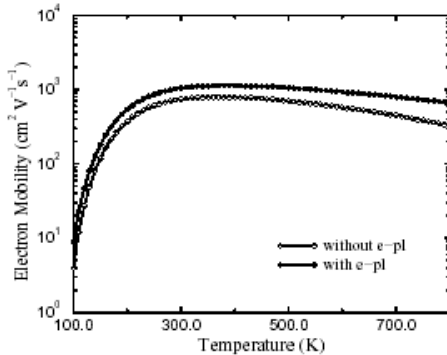

Fig.1: Calculated electron mobility in bulk ZnO as a function of temperature assuming a donor concentration of 10^{22} m^{-3} for the electron-plasmon scattering included and without the electron-plasmon scattering.

Fig. 2 shows the calculated variation of the electron mobility as a function of the donor concentration in bulk ZnO crystal structure at room temperature. The mobility does not vary monotonically between donor concentrations of 10^{21} m^{-3} and 10^{24} m^{-3} due to the dependence of electron-plasmon scattering on donor concentration, but shows a maximum near 10^{22} m^{-3} for both structures.
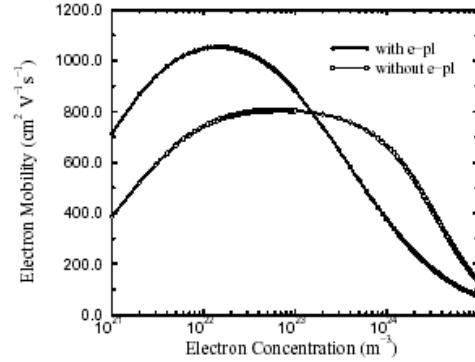

Fig.2: Calculated low-field electron drift mobility in ZnO as a function of different donor concentration at room temperature for the electron-plasmon scattering included and without the electron-plasmon scattering.

4. Conclusions

Using an iterative method, it was shown that the electron-plasmon scattering in the Γ valley substantially affects the electron mobility and transport properties in ZnO. It is shown that the electron mobility increase by 10%, and the Ohmic mobility drops by the same percent. This is caused by the combined effect of effective heating of electron gas by electron-plasmon scattering and the predominantly forward peaked momentum relaxation for all electron momenta.

References

[1] D. C. Look, Semicond. Sci. Technol. **20**, S55 (2005).
[2] A. Tsukazaki, A. Ohtomo, T. Onuma, M. Ohtani and M. Kawasaki, Nat. Mater. **4**, 42 (2005).
[3] T. Makino, Y. Segawa and A. Ohtomo, Appl. Phys. Lett. **78**, 1237 (2001).
[4] T. Makino, K. Tamura and C. H. Chia, Phys. Rev. B **65**, 121201(R) (2002).

[5]   E. Bellotti, B. K. Doshi and K. F. Brennan J. Appl. Phys. **85**, 916 (1999).

[6]   D. C. Look, D. C. Reynolds, J. R. Sizelove, and W. C. Harsch, Solid State Commun. **105**, 399 (1998).

[7]   Y. Chen, D. M. Bagnall, H. J. Koh, K. T. Park, Z. Q. Zhu and T. Yao, J. Appl. Phys. **84**, 3912 (1998).

[8]   C. Moglestue, *Monte Carlo Simulation of Semiconductor Devices* (Chapman and Hall, 1993).

[9]   C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor and Device Simulation* (Springer-Verlag, 1989).

[10] B. K. Ridley, *Electrons and Phonons in Semiconductor Multilayers* (Cambridge University Press, 1997).

[11] D. Chattopadhyay and H. J. Queisser, Review of Modern Physics **53**, part 1 (1981).

[12] K. Di. and K. Brennan, J. Appl. Phys. **69**, 3097 (1991).

[13] N. Mansour, K. Di. and K. Brennan, J. Appl. Phys. **70**, 6854 (1991).