Calculation of Electron Transport Properties in CdTe and HgCdTe at Low Electric Filed Application

[1]A. Haji Malekkheili, [2]N. Naghdiani, [3]K. Moradi Ankoochaksaraee and [4]G. H. Khorrami

[1]Department of Physics, Robat Karim Branch, Islamic Azad University, Tehran, Iran
[2]Department of Physics, Robat Karim Branch, Islamic Azad University, Tehran, Iran
[3]Department of Physics, Tehran Shomal Branch, Islamic Azad University, Tehran, Iran
[4]Department of Physics (Materials and Electroceramics Laboratory), Ferdowsi University of Mashhad, Mashhad, Iran

Abstract

Electron mobility in CdTe and HgCdTe are calculated, by solving Boltzmann equation using iteration model, as a function of temperature for carrier concentrations of 10^{16}, 10^{17}, and 10^{18} cm^{-3}. Both CdTe and HgCdTe have maximum mobility between 100 and 200 K, depending on the electron density. The theoretical maximum mobility in CdTe and HgCdTe at 300 K are about 1000 and 4400 $cm^2V^{-1}s^{-1}$. We compared the results with experimental data and find reasonable correlation.

Keywords-: Iteration Model; ionized impurity scattering; Electron mobilities.

I. INTRODUCTION

CdTe and HgCdTe semiconductors have been intensively investigated for last two decades for their potential applications in electronic, optoelectronic, and microelectronic device structures. The recent findings show that III-nitride semiconductors are also promising for nanostructure materials and nanodevices. The fabrication of homo and heterojunction devices mainly based on CdTe led to a rapid commercialization of light emitting diodes and laser diodes. The practical and commercial applications of these materials can be used in traffic lights, back lighting of mobile phones, indoor lights, light indicators for electronic devices, optical storage and display and solid state lasers. Another important application of these semiconductors is in fabrication of quantum infrared (IR) detectors. Photoconductors are the most common type of quantum IR detectors which can be fabricated by using nitride semiconductors [1]. 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 □ valley conduction band. We have also consider band non-parabolicity and the screening effects of free carriers on the scattering probabilities. All the relevant scattering mechanisms, including polar optic phonons, deformation potential, piezoelectric, acoustic phonons, and ionized impurity scattering. The Boltzmann equation is solved iteratively for our purpose, jointly incorporating the effects of all the scattering mechanisms [2-4].

This paper is organized as follows. Details of the iteration model , the electron scattering mechanism which have been used and the electron mobility calculations are presented in section II and the results of iterative calculations carried out on CdTe and HgCdTe structures are interpreted in section III.

II. MODEL DETAILS

To calculate 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,

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

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

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

Consider electrons in an isotropic, non-parabolic conduction band whose equilibrium Fermi distribution function is $f_0(k)$ in the absence of electric field. Note the equilibrium distribution $f_0(k)$ is isotropic in 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 *k* and *F* and *f₁(k)* is an isotropic function of *k*, which is proportional to the magnitude of the electric field. *f(k)* satisfies the Boltzmann equation 2 and it follows that,

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

(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*, $s_{eli}(k', k) = s_{eli}(k, k')$ equation 4 can be written as,

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

Note the first term in the denominator is simply the momentum relaxation rate for elastic scattering. Equation 5 may be solved iteratively by the relation,

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

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, 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 □ □, 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 GAN and InN structures using the iterative technique. In the following sections electron-phonon and electron-impurity scattering mechanisms will be discussed.

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 $2vk\hbar$, where v is the velocity of sound, since momentum conservation restricts the change of phonon wave vector to between zero and 2*k*, 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 order 10^5 cms^{-1}. Hence, $2vk\hbar$ ~ 1 meV, which is small 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 [2-5],

$$R_{de} = \frac{\sqrt{2}D^2{}_{ac}(m_t^{*2} m_l^{*})^{1/2} K_B T}{\pi\rho v^2 \hbar^4} \frac{\sqrt{E(1+\alpha E)}}{E(1+2\alpha E)} \qquad (8)$$
$$\left[(1+\alpha E)^2 + 1/3(\alpha E)^2\right]$$

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.

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. The piezoelectric scattering rate for an electron of energy *E* in an isotropic, parabolic band has been discussed by Ridley [4].
The expression for the scattering rate of an electron in a non-parabolic band structure retaining only the important terms can be written as [2-6]:

$$R_{PZ}(k) = \frac{e^2 K_B T K_{av}{}^2 \sqrt{m^*}}{2\sqrt{2}\pi\hbar^2\varepsilon_s}\gamma^{-1/2}(1+2\alpha\varepsilon)$$
$$\left[(1+\alpha\varepsilon)^2 + \frac{1}{3}(\alpha\varepsilon)^2\right] \qquad (9)$$

Where ε_s is the relative dielectric constant of the material and K_{av} is the dimensionless so called average electromechanical coupling constant.

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 is generally the most important scattering mechanism for electrons in III-V semiconductors, and this is also the case in CdTe and HgCdTe 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 [2-6],

$$R_{PO}(\vec{k}) = \frac{e^2\sqrt{2m^*}\,\omega_{PO}}{8\pi\varepsilon_\circ\hbar}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_\circ}\right)\frac{(1+2\alpha E)}{\sqrt{\gamma(E)}}$$

$$F_{PO}(E,E')\{N_{op}, N_{op}+1\} \quad (11)$$

Where $E = E' \pm hw_{po}$ is the final state energy phonon absorption (upper case) and emission (lower case) and *Nop* 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.

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 Coulombic interactions on their motion is increased. The electron scattering by ionized impurity centres has been discussed by Brooks Herring [5] who included the modification of the Coulomb potential due to free carrier screening. The screened Coulomb potential is written as,

$$V(r) = \frac{e^2}{4\pi\varepsilon_0\varepsilon_s}\frac{\exp(-q_0 r)}{r} \quad (12)$$

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

$$q_0{}^2 = \frac{ne^2}{\varepsilon_0\varepsilon_s K_B T} \quad (13)$$

Where n is the electron density. The scattering rate for an isotropic, non-parabolic band structure is given by [2-6],

$$R_{im} = \frac{N_i e^4(1+2\alpha E)}{32\sqrt{2m^*}\,\pi\,\varepsilon_s{}^2(\gamma(E))^{3/2}}\left[Ln(1+b) - \frac{b}{1+b}\right]$$

(14)

$$b = \frac{8m^*\,\gamma(E)}{\hbar^2 q_0^2} \quad (15)$$

Where N_i is the impurity concentration.

III. RESULTS

The electron mobility is a function of temperature and electron concentration .our results show that the electron mobility depends on total scattering in bulk CdTe and HgCdTe materials .Figures 1and 2 show total scattering depends on Energy , also increasing Temperature causes increasing total scattering in bulk CdTe and HgCdTe materials.

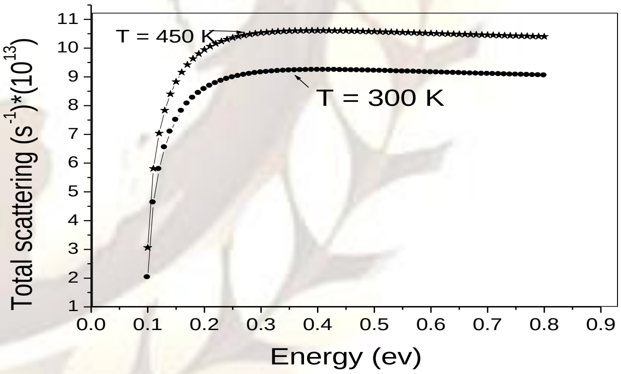

Fig 1. Changes total scattering electron Function in terms of energy in bulk CdTe at the different temperature.

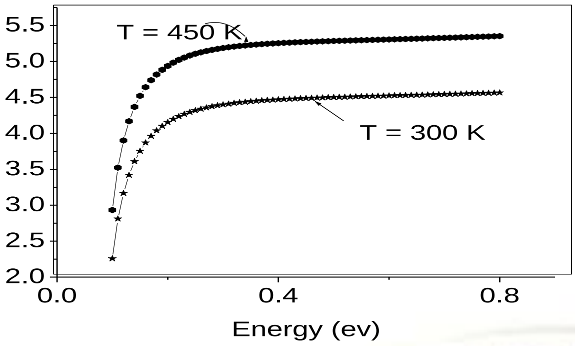

Fig 2. Changes total scattering electron Function in terms of energy in bulk HgCdTe at the different temperature.

Figure 3 shows the comparison totals scattering of CdTe and HgCdTe at the different temperature .our calculation results show that the totals scattering CdTe is more than HgCdTe .

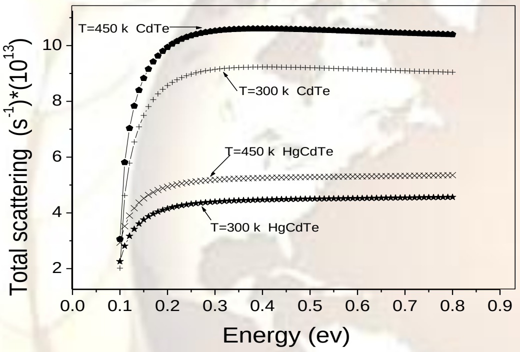

Fig 3. Changes total scattering electron Function in terms of energy in bulk CdTe and HgCdTe at the different temperature.

Figures 4 and 5 shows the electron mobility depends on the Temperature at the different electron concentration in bulk CdTe and HgCdTe materials.

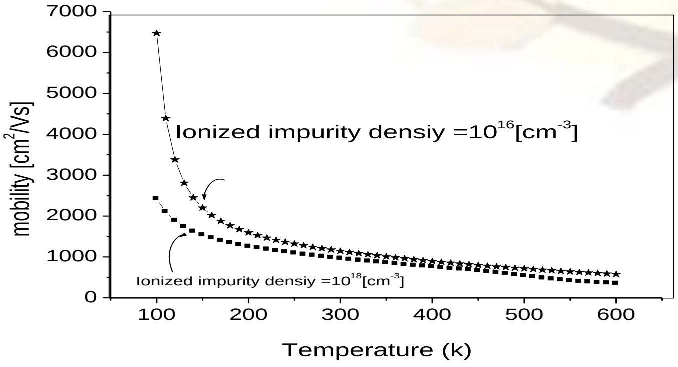

Fig 4. Changes the electron mobility Function in terms of temperature in bulk CdTe at the different electron concentration.

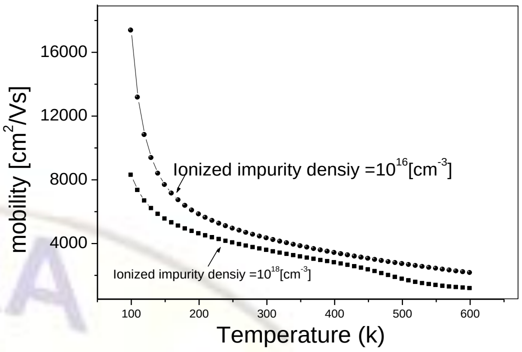

Fig 5. Changes the electron mobility Function in terms of temperature in bulk HgCdTe at the different electron concentration. figures 4 and 5 show that electrons mobility at the definite temperature 300 k for the CdTe semiconductors is gained about 1100cm^{2}v^{-1}s^{-1} and for HgCdTe about 4400 cm^{2}v^{-1}s^{-1}.also electrons mobility decrease quickly by temperature increasing from 100k to 600 k for all the different electron concentrations because temperature increasing causes increase of ponons energy too.so it causes a strong interaction between electrons and these ponons that its result is increase of electrons scattering rate and finally decrease of electrons mobility. Figure 6 shows comparison the electron mobility of CdTe and HgCdTe at the different electron concentration.our calculation results show that the electron mobility InN is more than GaN this increasing is because of small eff mass.

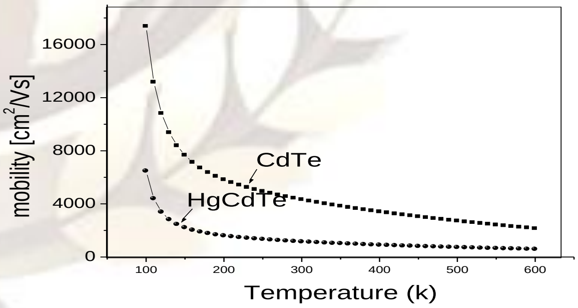

Fig 6. Changes the electron mobility Function in terms of temperature in bulk CdTe and HgCdTe at the electron concentration 10^{16} (cm^{-3}).

Figures 7 and 8 show the electron mobility depends on the electron concentration at the different Temperature in bulk CdTe and HgCdTe materials

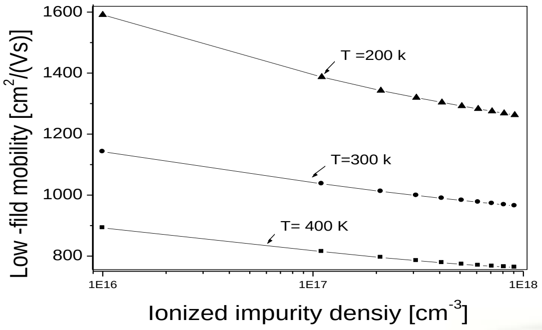

Fig 7. Changes the electron mobility Function in terms of electron concentration in bulk CdTe at the different Temperature.

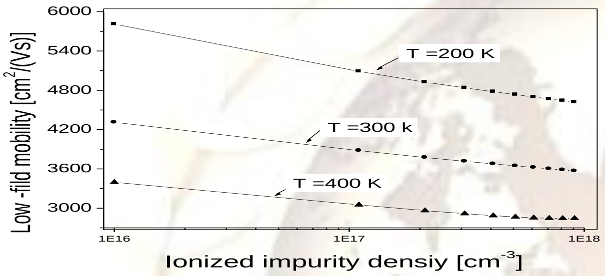

Fig 8. Changes the electron mobility Function in terms of electron concentration in bulk HgCdTe at the different Temperature

Figures 7 and 8 show that semiconductors mobility decrease by 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 9 shows comparison the electron mobility of CdTe and HgCdTe at the different Temperature .Our calculation results show that the electron mobility HgCdTe is more than CdTe

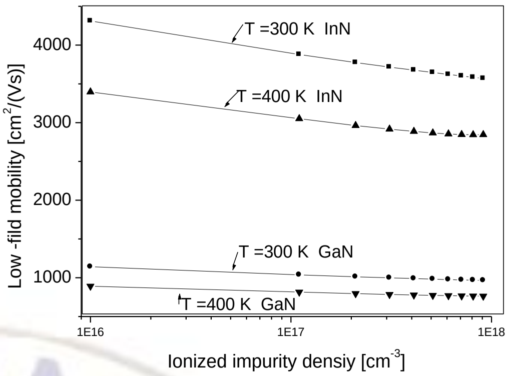

Fig 9. Changes the electron mobility Function in terms of electron concentration in bulk HgCdTe and at the different temperature.

IV. CONCLUSION

1. HgCdTe semiconductor having high mobility of CdTe because the effective mass is small compared with CdTe.
2. The ionized impurity scattering in both the semiconductor CdTe and HgCdTe at all temperatures is an important factor in reducing the mobility.

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