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Numerical Modeling of Carrier Transport Ratedue to Electrostatic InteractioninSemiconductor$Hg_{1-x}Cd_xTe$

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ABSTRACT: In this investigation,the carrier mobility forHgTe ,$Hg_{0.8}Cd_{0.2}Te$, CdTe structureshave been calculated by using numerical analysis in range of 77K-300K. we have been taking into account the spherical and parabolic band, elastic scattering of by piezoelectric scattering.The Boltzmann transport equation and the Fermi golden rule have been used.The electrons piezoelectric scattering rate, electrons and holes (heavy and light) piezoelectricmobility have been calculated as a function of different variables such as temperature and doping concentration. Calculations have been found that piezoelectricmobility ishigher for $Hg_{0.8}Cd_{0.2}Te$ than HgTe and CdTe,also the light hole piezoelectricmobility has been found that ishigher than the heavy hole piezoelectricmobility.

Keywords:Polar acoustic phonon, Piezoelectric, Carriers (electron and hole), Scattering, Mobility.

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I. INTRODUCTION

Nowadays the task of creation of fast and sensitivedetectors of THz spectral range based on HgCdTe is very important forvariousareas such as medicine, security, aerospace[1].Transportmechanisms have beenintensively investigated for the last two decades due to the advancement of technology fordetectors and microelectronic device in the infrared range [2]. Theelectron mobility is one ofthe most important parameters and importanttransport parameter used to determinetheperformance of devices[3].

In recent years Mercurycadmiumtelluride (MCT) structures are promisingmaterials for creation type of detectors.$Hg_{1-x}Cd_xTe$ components form a small direct band-gap zinc-blende system whose energy gap depends on alloy composition [1]. Keeping in mind its hugetechnological prospect, we need a betterunderstanding of these materials[4].

The purposeof the present paper is to calculate electron piezoelectric mobilityfor various temperatures and concentrations. Piezoelectric mobility is computed in the $Hg_{1-x}Cd_xTe$ semiconductor and compared with HgTe and CdTe.Most of the calculations have been carriedout using a non-parabolic ellipsoidal valley model todescribe transport inthe conduction band.However, the simpler and less computationally intensivespherical parabolic band scheme has also beenapplied, to test the validity of this approximation.

II. DETAILS MODEL

2.1. Materials and Procedures

In this paper ,the mobility of interactions with acoustic-polar (piezoelectric) phonons has been calculated ,Also we investigate electrons piezoelectricscattering and the carrierpiezoelectricmobility in $Hg_{1-x}Cd_xTe$semiconductor,it compared withHgTeandCdTe.

To calculate piezoelectricmobility, we have to solve The Boltzmann equation to get the modified probabilitydistribution function under the action of a steadyelectric field. Here, we have calculated the piezoelectricmobilityin $Hg_{1-x}Cd_xTe$structures using code written in MATLAB.The approximation of relaxation time, the Boltzmann transmission equation and the Fermi golden rule have been used.

2.2.Theelectron scattering rates by phonons (electrostatics interaction)

In polar compound semiconductors, optical phonons are associated with vibrating dipoles(whereatoms have some ionic charge).In addition, when acrystal does not have inversion symmetry, the strainassociated with acoustic phonons may produce apolarization field, with an electric field ofpiezoelectric nature, then the charge carrier scattering occurs due to the polar field of the longitudinalacoustic phonons of finite wavelengths. It happensa long-rangeelectrostatic interactionbetween electrons withphonons, is called polar interactions

and piezoelectric interactions respectively for optical phonons and acoustic phonons[5,6].

The first time the electron Scattering by piezoelectric phonons was investigated by Ridley [7,8], He considered electron scattering dueto piezoelectric elastic because of the low energy of the electrons. we have to determine the interaction energy of an electron with a potential field $\phi(r)$given by:

$$H_{ep} = \int \rho(r')\phi(r')\, d\,r'$$

where $\rho(r')$ is the electron charge density. Then, thisintegral is converted to using the Maxwell equation and Integration by parts yield:

$$H_{ep} = \int \varepsilon_\circ \nabla . E_e(r')\phi(r') d\,r' = -\varepsilon_\circ \int E_e(r').\nabla\phi(r') d\,r' = \varepsilon_\circ \int E_e(r').E_p(r') d\,r'$$

Where$E_e(r')$and$E_p(r')$respectively are the electric field associated with the electron charge and the electric field produced by the phonon. a screened Coulomb field produced by an electron in r′:

$$E_e(r') = -\frac{(-e)}{4\pi\varepsilon_\circ}\nabla_{r'}\left[\frac{1}{|r-r'|}e^{-q_\circ|r-r'|}\right]$$

wherethe inverse screening length this $q_\circ$. In the Debye equation, for nondegenerate statistics

$$q_\circ = \left[\frac{e^2 n}{\varepsilon KBT}\right]^{1/2}$$

where n is the electron density. Remember that $E_p(r')$, the field obtained bythe phonon, must distinguish betweenthe phonon modes.

2.3. The electron scattering rates byacousticphonons (piezoelectric Interaction)

Scattering by polar acoustic phonons is known as piezoelectric interactionThe polarization field in terms of the strain, Pi(**r**)is:

$$P_i(r) = \sum_{jk} e_{ijk}\frac{\partial y_j(r)}{\partial r_k}$$

Where $y_j(r)$ is the displacement field of the atoms associated withthe phonons

$$y_i(r) = \sum_{q,l} e_{ql}\left(\frac{\hbar}{2\rho V w_l(q)}\right)^{\frac{1}{2}}\{a_{ql} + a^{\dagger}_{-ql}\}e^{iqr}$$

where each mode is characterized by wavevector q, polarization e_{ql}, and angular frequency $w_l(q)$; ρ is the density of the crystal; a_{ql} and $a^{\dagger}_{-ql}$ are annihilation
and creation phonon operatorsand e_{ijk} is the piezoelectricconstant sothe strain tensor is

$$\frac{\partial y_i(r)}{\partial r_k} = \sum_{q,l}\left[(e_{ql})_j iq_k\right]\left(\frac{\hbar}{2\rho V w_l(q)}\right)^{\frac{1}{2}}\{a_{ql} + a^{\dagger}_{-ql}\}e^{iqr}$$

there is one independent constant in a zincblende structure (such as $Hg_{1-x}Cd_xTe$). e_{ijk} is a third-rank tensor and several elements of e_{ijk} are nonzero:
$e_{123} = e_{132} = e_{213} = e_{231} = e_{312} = e_{321}$.
Thefirst component of the polarization field is:

$$P_1(r) = e_{123}\left[\frac{\partial y_2(r)}{\partial r_3} + \frac{\partial y_3(r)}{\partial r_2}\right] = e_{123}\, i\sum_{q,l}\left[(e_{ql})_2 q_3 + (e_{ql})_3 q_2\right]\left(\frac{\hbar}{2\rho V w_l(q)}\right)^{\frac{1}{2}}\{a_{ql} + a^{\dagger}_{-ql}\}e^{iqr}$$

Following Maxwell equations, wehave

$$D = \varepsilon_\circ E + P$$

Where D is the electric induction fieldassociated with the phonon, that is zero, so the electric field associated with the acoustic phonon in the piezoelectric effect given by:

$$E_p(r) = -\frac{1}{\varepsilon_\circ}P_i(r)$$

now, inserting$P_1(r)$ into $E_p(r)$ then inserting $E_p(r)$ and $E_e(r')$into the Hamiltonian. This yield

$$H_{ep} = e_{123}\, i\int\left\{\frac{(-e)}{4\pi\varepsilon_\circ}\frac{\partial}{\partial r'_1}\left[\frac{1}{|r-r'|}e^{-q_\circ|r-r'|}\right]\right\} \times\left\{\sum_{q,l}\left[(e_{ql})_2 q_3 + (e_{ql})_3 q_2\right]\left(\frac{\hbar}{2\rho V w_l(q)}\right)^{\frac{1}{2}}\{a_{ql} + a^{\dagger}_{-ql}\}e^{iqr'}\right\}dr' + \cdots$$

$P_i(r)$ has three components, the dots indicate the products of the other components. Now we define a vector $\boldsymbol{a}(\boldsymbol{q},\boldsymbol{l})$, whose first component is$\left[(e_{ql})_2 q_3 + eql3q2\right.$, Then

$$H_{ep} = \frac{(-e)}{4\pi}\frac{1}{\varepsilon_\circ}\boldsymbol{e}_{123}\, i\sum_{\boldsymbol{q},\boldsymbol{l}}\left(\frac{\hbar}{\mathbf{2}\rho V w_l(q)}\right)^{\frac{1}{2}}\{\boldsymbol{a_{ql}} + \boldsymbol{a}^{\dagger}_{\boldsymbol{-ql}}\} \times \boldsymbol{a}(\boldsymbol{q},\boldsymbol{l}).\int \nabla_{r'}\left[\frac{1}{|r-r'|}e^{-q_\circ|r-r'|}\right]\boldsymbol{e}^{\boldsymbol{iq}r'}dr'$$

Then, using$r' - r = s$and then integrate by parts

$$I = \int \nabla_{r'}\left[\frac{1}{|r-r'|}e^{-q_\circ|r-r'|}\right]e^{iqr'}dr' = e^{iqr}\, iq\int\frac{1}{|s|}e^{-q_\circ|s|}e^{iqs}\,ds$$

To evaluate the integral above, wecan consider the polar coordinates, the result is

$$I = e^{iqr}\, iq4\pi\frac{1}{q}\frac{q}{q_\circ^2 + q^2}$$

Soequation H_{ep} becomes

H_{ep}

$$= -\frac{(-e)}{\varepsilon_\circ} e_{123} \sum_{q,l} a(q,l).q \left(\frac{\hbar}{2\rho V w_l(q)}\right)^{\frac{1}{2}} \frac{1}{q_\circ^2 + q^2} \{a_{ql} + a_{-ql}^{\dagger}\} e^{iqr}$$

For solve the aboveequation, an angular average over angles and phonon polarizations is convenient[8]:

$$H_{ep} = -\frac{(-e)}{\varepsilon_\circ} p \sum_{q,l} \left(\frac{\hbar}{2\rho V q v_s}\right)^{\frac{1}{2}} \frac{q^2}{q_\circ^2 + q^2} \{a_{ql} + a_{-ql}^{\dagger}\} e^{iqr}$$

where p and v_s are respectivelyaveraged piezoelectric constant and sound velocity.

The transition probability per unit time from a state$|k,c\rangle$ to a state$|k',c'\rangle$ reported by the Fermi golden rule

$$P(k,c;k',c') = \frac{2\pi}{\hbar} |\langle k',c'|H|k,c\rangle|^2 \delta(\epsilon(k',c') - \epsilon(\boldsymbol{k},c))$$

where $\epsilon(k,c)$ is the unperturbed energy of the state $|k,\rangle$ c, Then, the transition rate for the piezoelectric interactionbecomes:

$$P_a^{(p)}(k,k') = \frac{\pi p^2 e^2}{\rho V q v_s \varepsilon^2} \left(\frac{q^2}{q_\circ^2 + q^2}\right)^2 \begin{bmatrix} N_q \\ N_q + 1 \end{bmatrix} \mathcal{G}\delta[\epsilon(k') - \epsilon(k) \mp \hbar w_q]$$

Where $\mathcal{G}$ is the overlap integral and $N_q$is the number of phonons $q$in the state $|c\rangle$.

If elastic and equipartition approximations are made, the scatteringrate for the piezoelectric interaction where both absorption and emission are included

$$P_{ae}^{(p)}(k,k') = \frac{2\pi p^2 e^2 K_B T}{\hbar \rho V {v_s}^2 \varepsilon^2} \left(\frac{q}{q_\circ^2 + q^2}\right)^2 \delta[\epsilon(k') - \epsilon(k)]$$

Also, the overlap integral is taken to be unity and integrate over the possible final states

$$P_{ae}^{(p)}(k) = \frac{V}{(2\pi)^3} \int \frac{2\pi p^2 e^2 K_B T}{\hbar \rho V {v_s}^2 \varepsilon^2} \left(\frac{q}{q_\circ^2 + q^2}\right)^2 \delta[\epsilon(k') - \epsilon(k)] dk'$$

In a spherical andparabolic band, integration over the phonon wavevector yields:

$$P_{ae}^{(p)}(k) = \frac{1}{(2\pi)^2} \frac{p^2 e^2 K_B T}{\hbar \rho {v_s}^2 \varepsilon^2} \int \left(\frac{q}{q_\circ^2 + q^2}\right)^2 \delta\left[\frac{\hbar^2 (k \pm q)^2}{2m} - \frac{\hbar^2 k^2}{2m}\right] dq$$

we obtain thetransition rate as a function of electron energy [6,7], after calculations in polar coordinates with k as the polar axis

$$P_{ae}^{(p)}(\epsilon) = \frac{p^2 e^2 K_B T \sqrt{m}}{\sqrt{8}\pi\hbar^2 \rho {v_s}^2 k \varepsilon^2} \frac{1}{\sqrt{\epsilon}} \left[ln\left(1 + \frac{8m\epsilon}{\hbar^2 q_\circ^2}\right) - \frac{1}{\left(1 + \frac{\hbar^2 q_\circ^2}{8m\epsilon}\right)}\right]$$

Figure 1-3show the scattering rate by piezoelectric phonons as a function ofenergy, in$Hg_{0.8}Cd_{0.2}Te$, $CdTe$ and $HgTe$.

2.4. The electron mobility due to piezoelectric scattering

Assuming the elastic approximation with a relaxation time given by

$$\frac{1}{\tau_{ae}^{(p)}(\epsilon)} = \frac{V}{(2\pi)^3} \int \frac{2\pi p^2 e^2 K_B T}{\hbar \rho V {v_s}^2 \varepsilon^2} \left(\frac{q}{q_\circ^2 + q^2}\right)^2 \delta[\epsilon(k') - \epsilon(k)](1 - cos\,\theta) dk'$$

after integration,the result is

$$\frac{1}{\tau_{ae}^{(p)}(\epsilon)} = \frac{p^2 e^2 \sqrt{m} K_B T}{2\sqrt{2}\pi\hbar^2 \rho {v_s}^2 \varepsilon^2} \epsilon^{-\frac{1}{2}} \left[1 - \frac{\epsilon_o}{2\epsilon} log\left(1 + 4\frac{\epsilon}{\epsilon_o}\right) + \frac{1}{1 + 4\epsilon/\epsilon_o}\right]$$

the factor in square bracket is due to screening and can be approximated by

$$F_{PE} = \left[1 - \frac{\epsilon_o}{4K_B T} log\left(1 + \frac{8K_B T}{\epsilon_o}\right) + \frac{1}{1 + 8K_B T/\epsilon_o}\right]$$

by the F_{PE}constant, the mobility given by

$$\mu_{ae}^{(p)} = -\frac{16\sqrt{2\pi}}{3} \frac{\hbar^2 \rho {v_s}^2 \varepsilon^2}{p^2 e m^{3/2} \sqrt{K_B T} F_{PE}}$$

Figures4-6 the mobility due to piezoelectric scatteringin terms of temperature and figure 7-9 the mobility due to piezoelectric scatteringin terms ofElectron concentration, in $Hg_{0.8}Cd_{0.2}Te$, $CdTe$ and $HgTe$.

2.5. The heavy holemobility due to piezoelectric scattering

According to the Yadava, the longitudinal acoustic vibrations induce a dipolemoment per unit volume (polarization) Due to thepartly ionic nature of bonds in zinc-blende crystals.The heavy hole mobility in this case becomes

$$\mu_{hh}^{pz} = 25.43\, \varepsilon_s \left(\frac{m_{hh}}{m_o}\right)^{-3/2} K^{-2} T^{-1/2}$$

Where K is electro-mechanical coupling constant [10].

2.6. The light hole mobility due to piezoelectric scattering

According to the Kane band model, for large K values, the light hole band is non-parabolic. However, for smaller k near the band extremum, it can be approximated parabolicwith the density of states effective mass:

$$\frac{m_{hh}}{m_{lh}} = -\frac{1}{\left(1 - \frac{4m_0 P^2}{3\hbar^2 E_g}\right)}$$

P is an element of the Kane matrix and E_g the band gap, so we can calculate the light hole mobility of the by using the same formulas heavy hole after the exchange of m_{hh} with m_{lh} [10].

Figure 11-13theheavy andlight hole mobility due to piezoelectric scatteringin terms of temperatureinHg$_{0.8}$Cd$_{0.2}$Te,CdTeand HgTe.

III. RESULTS AND DISCUSSION

We have performed electron piezoelectric mobility calculations for calculating piezoelectricmobility, we have to solve the Boltzmann equation and considering the effect of dispersion electrons due to piezoelectricity.

Figures 1,2,3show the piezoelectric scattering rate depends on energy, in $Hg_{0.8}Cd_{0.2}Te$,CdTeand HgTeand structuresalso increasing temperature causes increasing scattering in materials.

Figures 4,5,6 show the electron piezoelectric mobilitydepends on the temperature at the different electronconcentration in materials,also electrons piezoelectric mobilitydecrease by temperature increasing for all the different electronconcentrations because temperature increasingcauses increase of phonons energy too, so it causes astrong interaction between electrons and thephonons that its result is an increase of electronspiezoelectric scattering rate and finally decrease of electronspiezoelectricmobility.

Figures7,8,9show the electron piezoelectric mobility dependson the electron concentration at the different temperatures 77,150,300 in$Hg_{0.8}Cd_{0.2}Te$,CdTeand HgTe me materialsthat semiconductors piezoelectric mobilitydecrease by electrons concentrations increasing because electrons increasing causes an increase of ionized impurity centers in crystals that it causestimes more electrons under the influence of the Coulomb potential of impurity centers located that its the result is an increase of electrons scattering rate andfinally, the decrease of electrons mobility.

Figure 10 shows,changes the electron piezoelectric mobility interms of temperature in $Hg_{0.8}Cd_{0.2}Te$,CdTeand HgTeat theelectronconcentration$10^{16}(cm^{-3})$. Ourcalculation results show that the electron piezoelectricmobility in $Hg_{0.8}Cd_{0.2}Te$is more than CdTeand HgTe.

Figures11,12,13 show the heavy and light hole piezoelectric mobility in terms oftemperaturein $Hg_{0.8}Cd_{0.2}Te$,CdTeand HgTematerials alsothe light hole piezoelectric mobility has been found that ishigher than the heavy hole mobility.

Fig. 1: The Scattering rate by piezoelectric phonons as a function of energy in $Hg_{0.8}Cd_{0.2}Te$.

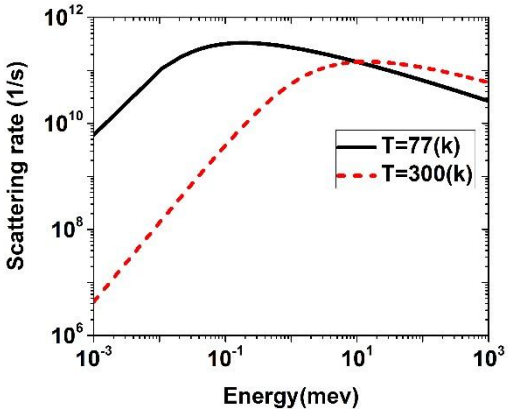


Fig. 2: The Scattering rate by piezoelectric phonons as a function of energy inCdTe.

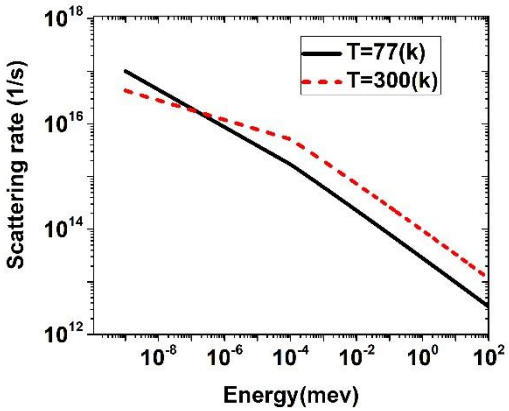


Fig. 3: The Scattering rate by piezoelectric phonons as a function of energy inHgTe.

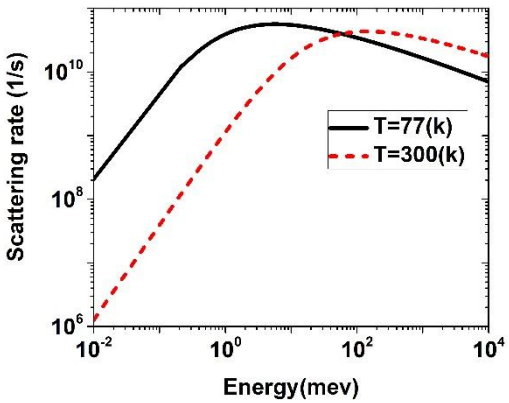


Fig. 4: The Mobility due to piezoelectric scattering in terms of temperature for $Hg_{0.8}Cd_{0.2}Te$.

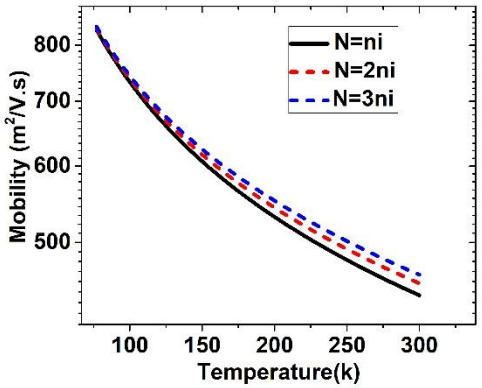


Fig. 5: The Mobility due to piezoelectric scattering in terms of temperature for CdTe.

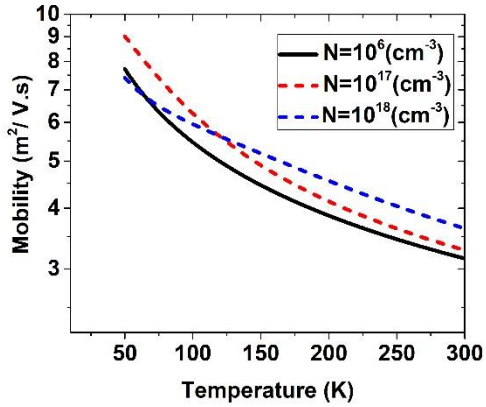


Fig. 6: The Mobility due to piezoelectric scattering in terms of temperature for HgTe.

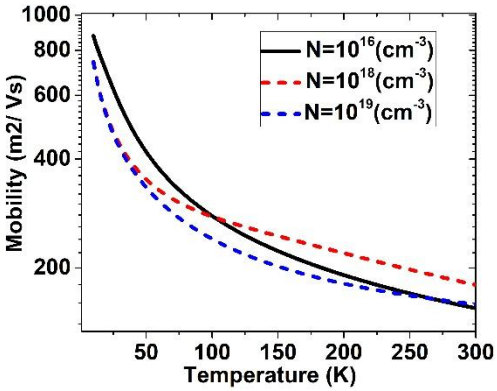


Fig. 7: The Mobility due to piezoelectric scattering in terms of electron concentration for $Hg_{0.8}Cd_{0.2}Te$.

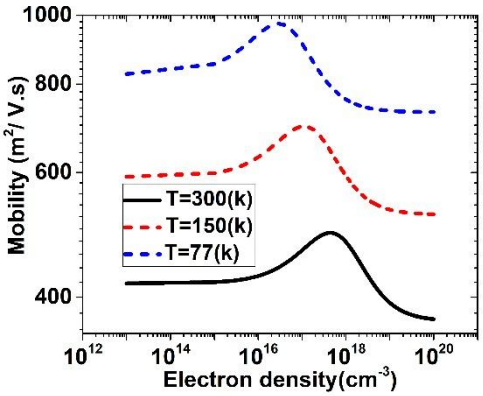


Fig. 8: The Mobility due to piezoelectric scattering in terms of electron concentrationforCdTe.

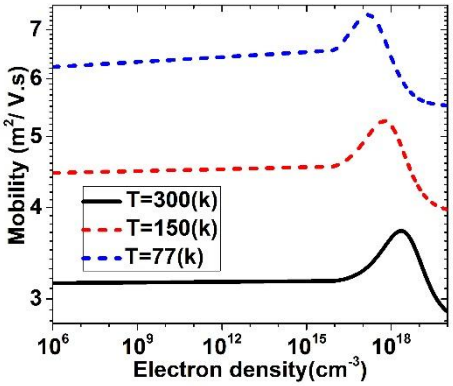


Fig. 9: The Mobility due to piezoelectric scattering in terms of electron concentration for HgTe.

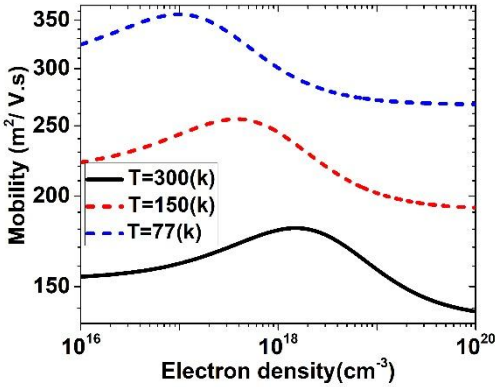


Fig. 10: The Mobility due to piezoelectric scattering in terms of temperature $Hg_{0.8}Cd_{0.2}Te$ (dot),CdTe(line) and (dash)HgTe with electron concentration 10^{16}.

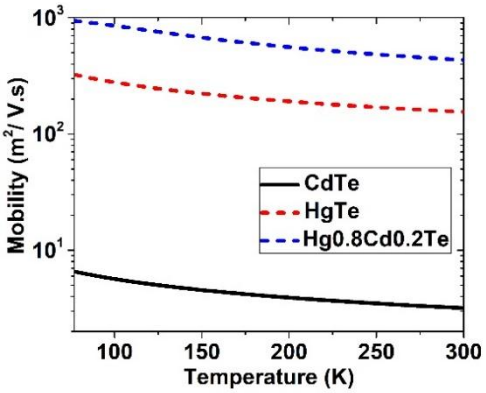


Fig. 11: The Heavy and Light Hole Mobility due to piezoelectric scattering in terms of temperature for$Hg_{0.8}Cd_{0.2}Te$.

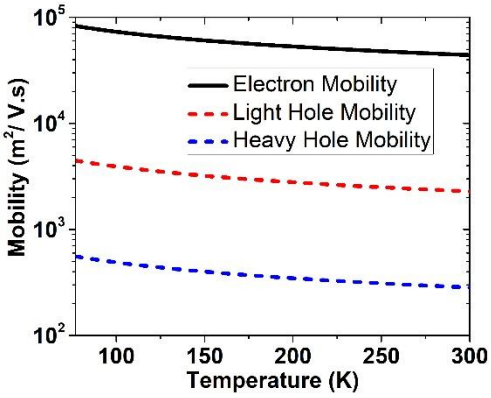


Fig. 12: The Heavy and Light Hole Mobility due to piezoelectric scattering in terms of temperaturefor CdTe-Electron(line), Light Hole(dash), Heavy Hole(dot)

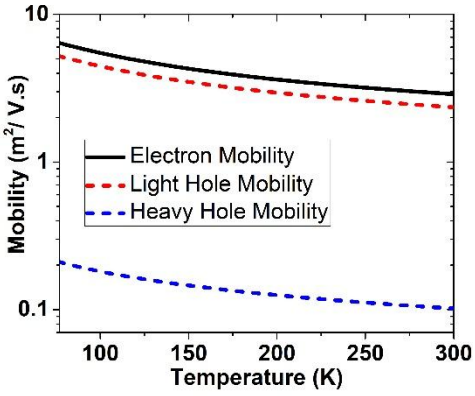
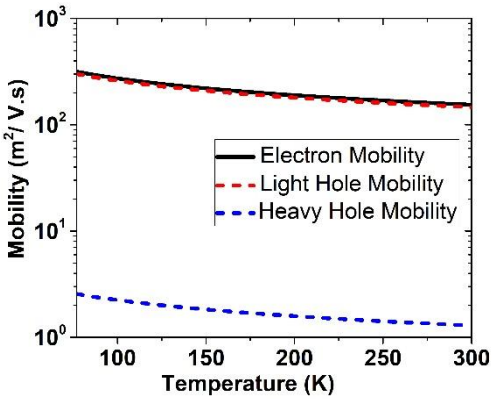


Fig. 13:The Heavy and Light Hole Mobility due to piezoelectric scattering in terms of temperaturefor HgTe. Electron(line), Light Hole(dash), Heavy Hole(dot)



CONCLUSION

In conclusion, we have quantitativelyobtainedtemperaturedependent and electronconcentration-dependent electron mobility in both$Hg_{0.8}Cd_{0.2}Te$,CdTeand HgTe. The theoretical values show good agreement with recently obtained experimental data.It has been found that mobility ishigher for $Hg_{0.8}Cd_{0.2}Te$ than HgTedue to the higher electron effective massin $Hg_{0.8}Cd_{0.2}Te$. The light hole mobility has been found that ishigher than the heavy hole mobility.

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