Longitudinal diffusivity in n-type $Hg_{0.8}Cd_{0.2}Te$ in the extreme quantum limit: Effect of alloy scattering

P. Banerji*
Department of Physics, University of Calcutta, 92 Acharya Prafulla Chandra Road, Calcutta-700 009, India

C. Chakraborty
Department of Electronics and Telecommunications Engineering, Jadavpur University, Calcutta-700 032, India

C. K. Sarkar†
Department of Physics, Bengal Engineering College, Shibpur, Howrah-711 103, India
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A theoretical model is proposed to study the effect of alloy scattering on the hot electron longitudinal diffusivity in n-type $Hg_{0.8}Cd_{0.2}Te$ in the extreme quantum limit, at a temperature of 4.2 K, assuming that the electron-electron interaction is strong enough to maintain a displaced Maxwellian distribution. It is seen that diffusivity increases with increase in electric field for all the scattering mechanisms, viz., ionized impurity scattering, alloy disorder, and polar-optic-phonon scatterings. Unlike in low-field transport where alloy disorder scattering is the most dominant mechanism, here polar-optic-phonon scattering is the most effective one. The effects of band hyperbolicity and free-carrier screening have also been examined. It is seen that when band hyparabolicity and quantum screening are included in the model, the theoretical value of the longitudinal diffusivity decreases. [S0163-1829(98)03023-9]

I. INTRODUCTION

The knowledge of diffusion constant for high field is important for understanding the device performance and operation. However, the Einstein relation for diffusion cannot be applied under the hot-electron condition because when high electric field is applied the diffusion current causes a first-order perturbation in the electron temperature and this in turn produces an additional variation in the current that is proportional to the concentration gradient. The behavior of electron diffusion in the presence of high field, therefore, is very much different from that at low fields. With the discovery of the quantum Hall effect, the studies on diffusive electron transport in low and high electric fields in the extreme quantum limit condition has emerged as an interesting field of research. Studies on diffusive transport show that it is related to the Fermi energy and to various other physical parameters. However, we have not come across any report on the study on the high-field diffusion constant in the extreme quantum limit magnetic fields.

In this article, a general mathematical model is proposed to calculate the hot-electron longitudinal diffusivity for nondegenerate electron statistics. This formulation has been applied to the case of $Hg_{0.8}Cd_{0.2}Te$ to examine the effect of alloy scattering on the hot electron diffusivity and then compare it with other scattering mechanisms and for various band structures.

II. THEORETICAL FORMULATION

The concentration gradient in a semiconductor may be produced from either inhomogeneity of the material or by external injection of charge carriers. When there is a variation in concentration, the carriers at any position experience a force proportional to the concentration gradient at that point. The drift velocity, resulting from this force, can be written as

$$V_d = -D\left(\frac{\delta n}{\delta z}\right)n^{-1}, \tag{1}$$

where D is diffusivity.

Let us consider the case of a semiconductor where the carrier concentration varies in the z direction and, say, the external electric field is also applied in the same direction. The Boltzmann transport equation for diffusion can then be written as[1]

$$\left(\frac{\hbar}{m^*}\right)k_z\left(\frac{\delta f}{\delta z}\right)+\left(\frac{e}{\hbar}\right)\mathcal{E}\left(\frac{\delta f}{\delta k_z}\right)+\left(\frac{\delta f}{\delta t}\right)=\left(\frac{\delta f}{\delta t}\right)_{\text{coll}}, \tag{2}$$

where m^* is the effective mass, k_z is the z component of the electron wave vector, $\hbar$ is Planck's constant divided by 2π, e is the electronic charge, $\mathcal{E}$ is the electric field, and f is the distribution function given by[2]

$$f(z,k_z,t)=f_0(z,E,t)+k_z f_1(z,E,t). \tag{3}$$

Equation (2) can also be applied when a magnetic field is present. Let us assume that the magnetic field is also applied along the z direction. The expression for energy in the presence of a quantizing magnetic field is then

$$E=\frac{\hbar^2 k_z^2}{2m^* a_0}+(n+1/2)\hbar\omega_c-\frac{E_g a_0}{2}, \tag{4}$$

where a_0 measures the nonparabolicity and it approaches unity in the wide band-gap limit. The expression for a_0 can be written as

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$$a_0=\left[1+\frac{2\hbar\omega_c}{E_g}\left(1-|g|\frac{m^*}{2m_0}\right)\right]^{1/2}, \tag{5}$$

where E_g is the band gap, $\omega_c=eB/m^*$, $|g|$ is the Landé g factor, and m^* and m_0 are the band-edge effective and free-electron masses respectively.

Recent studies on scattering mechanisms by Krishnamurthy and Sher[3] and by Chen and Sher[4] gradually manifested on the idea of considering the hyperbolic band structure to minimize the deviation between the theory and experiment stimulate us to take the hyperbolic band energy expression as

$$E=(\gamma k^2+c^2)^{1/2}-c \tag{6}$$

with $k^2=(n+\frac{1}{2})(2eB/\hbar)+k_z^2$ and the corresponding reduced mass is obtained from $1/m^*=(1/\hbar^2k)(\delta E/\delta k_z)$. The terms γ and c are adjusted to fit the calculated band structure in the energy range of interest.

Using Eqs. (3) and (4) in Eq. (2) we get

$$f_1=-\left(\frac{\hbar}{m^*}\right)\tau(E)\left[\frac{\delta f_0}{\delta z}+e\mathcal{E}\frac{\delta f_0}{\delta E}\right], \tag{7}$$

where $\tau(E)$ is the relaxation time obtained from the corresponding scattering mechanism.

The current density is

$$J=\int eV_z dn, \tag{8}$$

$$=\int_{-\infty}^{\infty}\frac{e}{\pi m^* a_0}(f_0+k_z f_1)k_z dk_z$$

$$=\frac{2e}{\pi m^* a_0}\int_0^{\infty}k_z^2 f_1 dk_z. \tag{9}$$

Making use of Eq. (4) and expression for f_1 from Eq. (7) in Eq. (9) we get,

$$J=-\frac{8^{1/2}m^* a_0 e}{\pi^2}\left(\frac{\hbar}{m^*}\right)\int_0^{\infty}\tau(E)E^{1/2}\left[\frac{\delta f_0}{\delta z}+e\mathcal{E}\frac{\delta f_0}{\delta E}\right]dE. \tag{10}$$

The perturbation on the distribution function would be small if a small concentration gradient is taken. Hence

$$f_0=f_0^0(n,E)+1/n\frac{\delta n}{\delta z}f_0^1(n,E), \tag{11}$$

where f_0^0 is the heated Fermi-Dirac distribution function.

Using Eq. (11) in Eq. (10) we can write

$$J=-\frac{8^{1/2}a_0 e}{\pi m^{*1/2}}\int_0^{\infty}\tau(E)E^{1/2}\left[\frac{\delta f_0}{\delta z}+e\mathcal{E}\left(\frac{\delta f_0^0}{\delta E}+1/n\frac{\delta n}{\delta z}\frac{\delta f_0^1}{\delta E}\right)\right]dE$$

$$=\frac{8^{1/2}a_0 e^2\mathcal{E}}{\pi m^{*1/2}}\int_0^{\infty}\tau(E)E^{1/2}\frac{\delta f_0^0}{\delta E}dE$$

$$-\frac{8^{1/2}a_0 e}{\pi m^{*1/2}}\int_0^{\infty}\tau(E)E^{1/2}\left[\frac{\delta f_0}{\delta E_F}\frac{\delta E_F}{\delta n}+\frac{e\mathcal{E}}{n}\frac{\delta f_0^1}{\delta E}\right]dE\left(\frac{\delta n}{\delta z}\right). \tag{12}$$

Comparing the above equation with

$$J=n_0 e\mu\mathcal{E}-eD_L\frac{\delta n}{\delta z}, \tag{13}$$

we get

$$\mu=-\frac{8^{1/2}a_0 e}{\pi m^{*1/2}n_0}\int_0^{\infty}\tau(E)E^{1/2}\frac{\delta f_0^0}{\delta E}dE, \tag{14}$$

$$D_L=\frac{8^{1/2}a_0}{\pi m^{*1/2}}\int_0^{\infty}\tau(E)E^{1/2}\frac{\delta f_0}{\delta E_F}\frac{\delta E_F}{\delta n}dE$$

$$+\frac{8^{1/2}a_0 e\mathcal{E}}{\pi m^{*1/2}n_0}\int_0^{\infty}\tau(E)E^{1/2}\frac{\delta f_0^1}{\delta E}dE. \tag{15}$$

Then the expression for longitudinal diffusivity comes out as

$$D_L=\frac{n_0\mu}{e}\frac{\delta E_F}{\delta n}+\frac{8^{1/2}a_0 e\mathcal{E}}{\pi m^{*1/2}a_0}\int_0^{\infty}\tau(E)E^{1/2}\frac{\delta f_0^1}{\delta E}dE. \tag{16}$$

The term $(\delta E_F/\delta n)$ in Eq. (16) can be replaced by k_BT/n for hyperbolic band structure and the integration can be replaced by

$$\frac{1}{kT}\int_0^{\infty}\tau(E)E^{1/2}\exp(-E)dE \tag{17}$$

for nondegenerate semiconductors.

When an electric field is applied parallel to the applied magnetic field, the electrons gain energy from the electric field and the temperature of the electron system increases. The difference between the electron temperature and the lattice temperature becomes large, causing the electrons to emit more phonons than they absorb at higher electric fields. A balance is needed to achieve a steady state where the energy input into the electronic system at a given field and the energy loss from the carriers are equal.

We first calculate the average energy loss rate per electron through emission and absorption of acoustic and polar-optic phonons, the details of which have been deduced elsewhere.[5,6] The acoustic-phonon scattering via deformation potential as well as via piezoelectric coupling has been neglected because it contributes little, to the energy-loss mechanism. In calculating the energy-loss rate for acoustic-phonon scattering via the deformation potential, the phonon occupation number is assumed to be independent of electric field and is given by Bose-Einstein statistics. The effect of phonon disturbance on the drift velocity due to lattice heating has been neglected because of the large wave-vector acoustic phonon in the extreme quantum limit.[2]

The electric field is given by the relation

$$\mathcal{E}=\left(\frac{P}{e\mu}\right)^{1/2}, \tag{18}$$

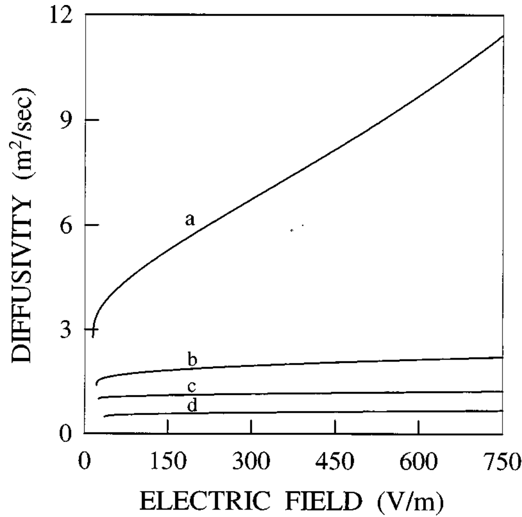

FIG. 1. Variation of the hot electron longitudinal diffusivity in n-type $Hg_{0.8}Cd_{0.2}Te$ in the extreme quantum limit at 4.2 K for a magnetic field of 4 T for different scattering mechanisms (curve a for ionized impurity, curve b for alloy, curve c for polar optic phonon, and curve d for all scattering) at a magnetic field of 4 T.

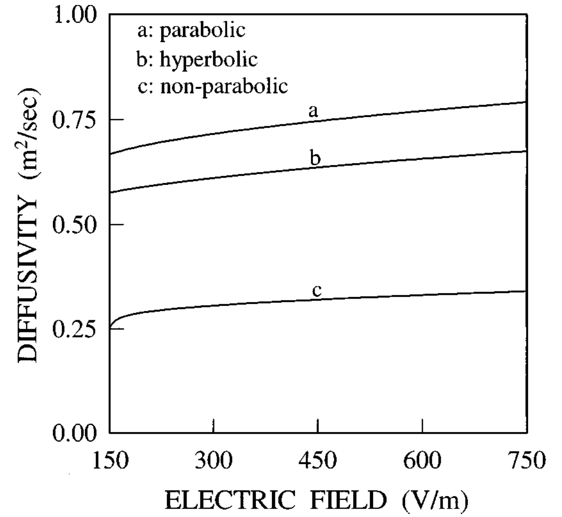

FIG. 2. Electric-field dependence of the hot-electron longitudinal diffusivity in n-$Hg_{0.8}Cd_{0.2}Te$ in the extreme quantum limit at 4.2 K and magnetic field 4 T due to different band structures.

where P is the energy-loss rate and μ is the mobility and its value is calculated from the momentum relaxation times of carriers.[7]

When a large electric field is applied, the velocity of the electrons becomes higher than the thermal velocity corresponding to the lattice temperature. The electron energy is transferred to the lattice through the carrier scattering mechanisms. In the presence of a quantizing magnetic field, electron-electron interaction in a bulk material is stronger than that without a magnetic field due to quantum confinement effect and also due to the weakness of ionized impurity scattering in high magnetic fields. It can be assumed that the electron-electron interaction is strong enough to maintain a displaced Maxwellian distribution of carriers. The physical condition required for the distribution to be a displaced Maxwellian[8] implies that the sample should have a critical electron concentration of about 10^{15} cm^{-3}. The drift velocity of carriers in the high-electric-field region is assumed to be proportional to the applied electric field with the electron mobility as the constant of proportionality. This assumption is justified in the high-electric-field condition, where the electron temperature model is considered. In the extreme quantum limit, the electron temperature model is used for electron gas because strong electron-electron interaction caused by the magnetic confinement as observed in the low-dimensional electron system[9] prevails in this case. The high electric field affects the mobility through the relaxation time τ or the effective mass m^* (for nonparabolic band semiconductors), both being functions of electron temperature.[1]

So far as the intervalley scattering mediated by alloy disorder is concerned this can be neglected in the present case. The mobility in the lower valley (μ_l) is much larger than that in the higher valleys (μ_h). Assuming $\mu_l \gg \mu_h$, the drift velocity can be approximated by[10]

$$V_d = \frac{\mu_l \mathcal{E}}{1 + R\exp[-\Delta\mathcal{E}/(k_B T_e)]}, \tag{19}$$

where R is the ratio of the densities of states in the upper to the lower valleys, respectively, and $\Delta\mathcal{E}$ is the energy differences between the minima of these two valleys. V_d is very small in our case and so can be neglected.

III. RESULTS AND DISCUSSION

The longitudinal diffusivity has been calculated in n-$Hg_{0.8}Cd_{0.2}Te$ using the material parameters taken from Refs. 1 and 11 at 4.2 K. The integration part of the right-hand side of Eq. (16) has been worked out numerically. The values of relaxation times $\tau(E)$ have been calculated using the expressions given in Ref. 7 at a magnetic field of 4 T. The longitudinal diffusivity has been calculated using the acoustic-phonon scattering, ionized impurity, alloy disorder, and polar-optic-phonon scatterings.

The theoretically calculated values of longitudinal diffusivity are plotted against the electric field in Fig. 1 for dif-

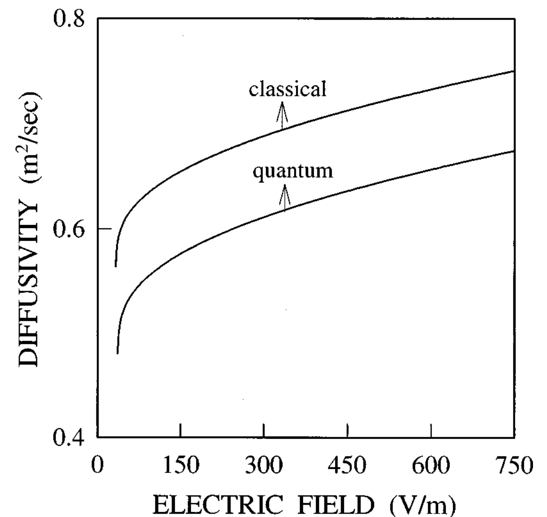

FIG. 3. Variation of the hot-electron longitudinal diffusivity in n-$Hg_{0.8}Cd_{0.2}Te$ in the extreme quantum limit at a magnetic field of 4 T at 4.2 K for a different screening.

ferent scattering mechanisms at a magnetic field of 4 T considering the hyperbolic nature of the conduction band. It is seen from the figure that, in general, diffusivity increases with the electric field except in the case of ionized impurity scattering when the increase is very sharp. Since ionized impurity scattering is coulombic in nature, its efficiency decreases with increase in electric field and gives rise to such a behavior. Here, polar-optic-phonon scattering is the most dominant scattering mechanism, in contrast to the low-field condition where alloy scattering is the most effective one.

The longitudinal diffusivity is plotted against the electric field in Fig. 2 for different band structures at a temperature of 4.2 K. It is seen that diffusivity attains a higher value for the case of hyperbolic band, whereas inclusion of band nonparabolicity decreases the diffusivity. The band nonparabolicity increases the scattering rate and also increases the energy dependent effective mass of conduction electrons and thereby decreases the diffusivity as also observed in experimental case.[9]

The screening of the carriers also affect the diffusivity as shown in Fig. 3 where the electric-field dependence of the diffusivity is shown. It is seen from this figure that the diffusivity, when the quantum nature of the free-carrier screening is considered, is less than that when classical screening is considered. In the extreme quantum limit, the electrons occupy only the lowest Landau level since the magnetic field is assumed to be very strong, i.e., $\hbar\ \omega_c \gg k_B T$. However, the application of a magnetic field, however strong it may be, cannot provide the energy necessary to redistribute the shielding charges. It is the quantum nature of the free-electron gas that gives rise to the effect due to magnetic field. This is due to the noncommutation of the free-carrier Hamiltonian associated with the potential of the scattering centers. According to the low-field measurement of the heat capacity of n-$Hg_{0.8}Cd_{0.2}Te$ by Nimtz and Gebhardt,[12] the electrons in the system behave as a nondegenerate electron gas in the magnetic quantum limit where only one degree of freedom of translational motion is left. The screening parameter, thus, is modified due to the one-dimensional density of states caused by magnetic quantization. The effect of quantization is to reduce the inverse quantum screening length compared to the (inverse) Debye screening length. The inclusion of magnetic-field-dependent screening in the scattering matrix increases the scattering rate and hence decreases the diffusivity.

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[*]Present address: Materials Science Center, Indian Institute of Technology, Kharagpur-721 302, India. Electronic address: pallabb@matsc.iitkgp.ernet.in

[†] On leave from ETCE Department, Jadavpur University, Calcutta 700 032, India.

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