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Magnetoelectronic transport of the two-dimensional electron gas in CdSe single quantum wells

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Abstract. Hall mobility and magnetoresistance coefficient for the two-dimensional (2D) electron transport parallel to the heterojunction interfaces in a single quantum well of CdSe are calculated with a numerical iterative technique in the framework of Fermi–Dirac statistics. Lattice scatterings due to polar-mode longitudinal optic (LO) phonons, and acoustic phonons via deformation potential and piezoelectric couplings, are considered together with background and remote ionized impurity interactions. The parallel mode of piezoelectric scattering is found to contribute more than the perpendicular mode. We observe that the Hall mobility decreases with increasing temperature but increases with increasing channel width. The magnetoresistance coefficient is found to decrease with increasing temperature and increase with increasing magnetic field in the classical region.

Keywords. CdSe quantum wells; 2D electron gas; magneto-electronic transport.

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1. Introduction

The transport properties of two-dimensional (2D) electron gas in ZnTe/CdSe single quantum wells (QWs) have assumed considerable importance of late owing to their scientific importance and technological applications, particularly in optoelectronic devices [1,2]. As the width of the QW is comparable to the de Broglie wavelength, a sub-band structure of electron energy levels is formed and the electrons in the QW itinerate two-dimensionally parallel to the heterojunction interfaces. Detailed studies on magnetoelectronic transport in CdSe QWs have not yet been reported in the literature. In this paper, we calculate the Hall mobility and the magnetoresistance coefficient of the 2D electron gas in a CdSe single QW for nonquantizing magnetic

fields incorporating the Fermi–Dirac distribution function with a numerical iterative technique. We include lattice scattering of the 2D electrons via polar-mode longitudinal optic (LO) phonons and acoustic phonons through deformation potential and piezoelectric interactions. We also incorporate scattering by remote and background ionized impurities. We study here the effects of the variation of temperature, channel width, and the magnetic field on the transport coefficients of the CdSe single QW.

2. Analytical details

The band gaps of ZnTe and CdSe are 2.34 eV and 1.75 eV, respectively. As in AlAs/GaAs QWs, the conduction band offset in the ZnTe/CdSe single QWs is taken to be 60% of the difference of the band gaps. As such, the conduction band offset for the ZnTe/CdSe QWs is about 0.36 eV, which is more than 16 times the maximum value of the Fermi energy $E_{\rm F}$ of the 2D electrons of concern here. Thus the CdSe square well can be assumed to be infinite. Also, the electrons here are confined to the lowest sub-band since the next higher sub-band is about $4E_{\rm f}$ high in energy above the lowest sub-band. These approximations lead to tractable analytical expressions befitting many problems of practical interest.

In the rectangular Cartesian coordinate system, we assume that the z-axis is perpendicular to the heterojunction interfaces so that the 2D transport occurs parallel to the interfacial xy-plane. An electric field $\mathbf{F}$ is assumed to act along the x-axis and a nonquantizing magnetic field $\mathbf{B}$ along the z-axis. In the crossed fields, the electrons experience an electromagnetic force so that the distribution function is perturbed in the direction of $\mathbf{F}$, and also in the direction perpendicular to both $\mathbf{F}$ and $\mathbf{B}$. Hence, in the single-band effective mass approximation, the electron distribution function can be written as [3,4]

$$f(\mathbf{k}) = f_0(E) + [e\hbar F/m^*][k_x\xi_x(E) - \omega_{\rm c}k_y\xi_y(E)]\left(-\frac{\partial f_0}{\partial E}\right), \tag{1}$$

where $\mathbf{k}$ is the 2D wave vector of the electron of energy E measured from the sub-band minimum, $f_0(E)$ is the equilibrium Fermi–Dirac distribution function, e and m^* are the charge and the effective mass of an electron, $\hbar$ is the Planck's constant divided by 2π, k_x and k_y are the x- and y-components of $\mathbf{k}$, respectively, and $\omega_{\rm c}(= eB/m^*)$ is the cyclotron resonant frequency. $\xi_x(E)$ is the perturbation function in the x-direction, i.e., in the direction of $\mathbf{F}$, and $\xi_y(E)$ is the perturbation function in the y-direction, i.e., in the direction transverse to both $\mathbf{F}$ and $\mathbf{B}$. These perturbation functions determine the magnetoelectronic transport coefficients of interest here.

The Boltzmann transport equation for the problem is [4]

$$\left[\frac{eF}{\hbar} + \omega_{\rm c}k_y\right]\frac{\partial f}{\partial k_x} - \omega_{\rm c}k_x\frac{\partial f}{\partial k_y} = \left(\frac{\partial f}{\partial t}\right)_{\rm coll}, \tag{2}$$

where $(\partial f/\partial t)_{\rm coll}$ represents the time rate of change of $f(\mathbf{k})$ due to the scattering processes. We substitute for $f(\mathbf{k})$ from eq. (1) in eq. (2) and use the relevant

expressions for the scattering rates [5]. Ignoring the small-order terms and equating the coefficients of k_x and k_y from the two sides of the resulting equation, we obtain the following two coupled equations for the perturbation functions $\xi_x(E)$ and $\xi_y(E)$:

$$[S_0(E) + 1/\tau(E)]\xi_x(E) = 1 + S_+(E)\xi_x(E + \hbar\omega) + S_-(E)\xi_x(E - \hbar\omega) - \omega_c^2\xi_y(E) \quad (3)$$

and

$$[S_0(E) + 1/\tau(E)]\xi_y(E) = \xi_x(E) + S_+(E)\xi_y(E + \hbar\omega) + S_-(E)\xi_y(E - \hbar\omega). \quad (4)$$

Here, $S_0(E)$ is the scattering rate out of the state with energy E due to the absorption and emission of LO phonons of energy $\hbar\omega$, and $S_+(E)$ and $S_-(E)$ denote the scattering rates into the state with energy E due to the emission and absorption of LO phonons, respectively [5,6]. $1/\tau(E)$ is the combined momentum relaxation rates due to the elastic scattering processes, viz., acoustic scattering via deformation potential and piezoelectric couplings, and screened Coulomb scattering via background and remote ionized impurities. The expressions for these rates are obtained from Chattopadhyay [5]. Note that these rates depend on the width of the QW, i.e. the channel width L_z. Also, the scattering rates are not affected by the magnetic field in the classical region [4].

The piezoelectric coefficient is isotropic for the sphalerite crystal and anisotropic for the wurtzite crystal. This results in the two piezoelectric relaxation rates $1/\tau_{\perp\mathrm{p}}$ and $1/\tau_{\parallel\mathrm{p}}$ for the different piezoelectric coefficients for the electric field perpendicular and parallel to the c-axis in CdSe [6].

Equations (3) and (4) are solved for $\xi_x(E)$ and $\xi_y(E)$ with a numerical iterative technique. In the ith step of iteration, $\xi_x(E)$ and $\xi_y(E)$ are determined by using in the right-hand sides of eqs (3) and (4) the values of $\xi_{x,y}(E \pm \hbar\omega)$ obtained in the $(i-1)$th step. In the first step, $\xi_{x,y}(E \pm \hbar\omega)$ are put to zero. About seven iteration steps are needed to obtain convergent results.

The Hall mobility μ_H and magnetoresistance coefficient R_m are given by [7]

$$\mu_\mathrm{H} = \mu_{xx}(0)|\mu_{xy}|/[B(\mu_{xx}^2 + \mu_{xy}^2)] \quad (5)$$

and

$$R_\mathrm{m} = \mu_\mathrm{H} B\mu_{xx}/|\mu_{xy}| - 1, \quad (6)$$

where

$$\mu_{xx} = \frac{e}{\pi N_\mathrm{2D}\hbar^2}\int_0^\infty E\xi_x(E)\left(-\frac{\partial f_0}{\partial E}\right)\mathrm{d}E$$

and

$$\mu_{xy} = \frac{e\omega_c}{\pi N_\mathrm{2D}\hbar^2}\int_0^\infty E\xi_y(E)\left(-\frac{\partial f_0}{\partial E}\right)\mathrm{d}E.$$

The quantity $\mu_{xx}(0)$ is the value of μ_{xx} for $B = 0$ and N_2D is the 2D electron concentration in the QW.

Table 1. Material parameters of CdSe used in the calculations.

Parameters	Values
Static dielectric constant	9.4
Optic dielectric constant	6.1
Longitudinal elastic constant	7.37×10^{10} N m^{-2}
Transverse elastic constant	2.459×10^{10} N m^{-2}
Acoustic deformation potential constant	3.7 eV
Piezoelectric tensor component for parallel mode scattering	3.37×10^{9} V m^{-1}
Piezoelectric tensor component for perpendicular mode scattering	2.36×10^{9} V m^{-1}
Polar LO phonon temperature	303 K

3. Results and discussion

The effective mass of the electrons for CdSe including polaronic correction is $m^* = 0.12m_0$, where m_0 is the electron rest mass [2]. The other parameter values related to CdSe and used in our calculations, are taken from Rode [6] and given in table 1.

In figure 1, $\mu_\parallel$ and $\mu_\perp$ are the calculated Hall mobilities with piezoelectric parallel mode and perpendicular mode scatterings, respectively, incorporating all other scattering processes. The variations of these mobilities are displayed over the temperature range of 30 to 300 K for a typical channel width $L_z = 10.5$ nm and a typical 2D carrier concentration $N_{2D} = 4.8 \times 10^{15}$ m^{-2} with $B = 0.002$ T. The ionized impurity concentration is taken as $N_i = 8.6 \times 10^{22}$ m^{-3} which fits the experimental mobility at 4.2 K reported by Ng *et al* [2]. The phonon occupation numbers and hence the lattice scattering rates increase with increasing temperature, forcing the mobility to decrease as the temperature rises. The ionized impurity scattering rate increases with decreasing temperature since this scattering is Coulombic in nature. As a result, the drop of mobility with increasing temperature on the low-temperature side is somewhat weakened. The piezoelectric scattering rate is stronger for parallel mode than for the perpendicular mode. So, $\mu_\perp$ is found to be higher than $\mu_\parallel$ by 46% at 30 K and by 22% at 300 K. The lesser effect of the anisotropy of the piezoelectric scattering on the mobility at 300 K is accounted for by the preponderance of the LO phonon scattering there. No appreciable change in the mobility is observed as B is increased from 0.002 T to 0.02 T.

Due to the lack of experimental data at present, reflecting the effects of parallel and perpendicular modes of piezoelectric scattering, we include only the former in the remaining calculations to study the parameter dependences of the transport coefficients. Although the numerical values of the coefficients will change somewhat, the nature of the curves will remain the same as the piezoelectric scattering changes to the perpendicular mode.

Figure 2 shows the dependence of the Hall mobility on the channel width L_z at 30, 77, and 300 K. The values of the other material parameters used to obtain the curves in figure 2 are the same as those used for figure 1. The mobilities are found to remain insensitive to the change in the magnetic field from 0.002 T to 0.02 T, as

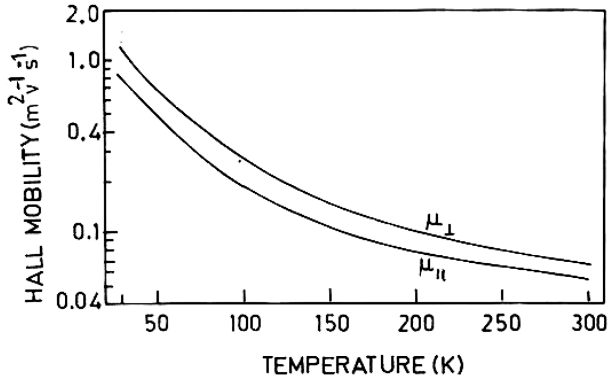

Figure 1. Temperature variation of Hall mobility for $L_z = 10.5$ nm, $N_{2D} = 4.8 \times 10^{15}$ m^{-2}, $N_i = 8.6 \times 10^{22}$ m^{-3}, and $B = 0.002$ T. $\mu_{||}$ and $\mu_\perp$ represent mobilities with piezoelectric parallel mode and perpendicular mode scatterings, respectively, and including all other scattering mechanisms.

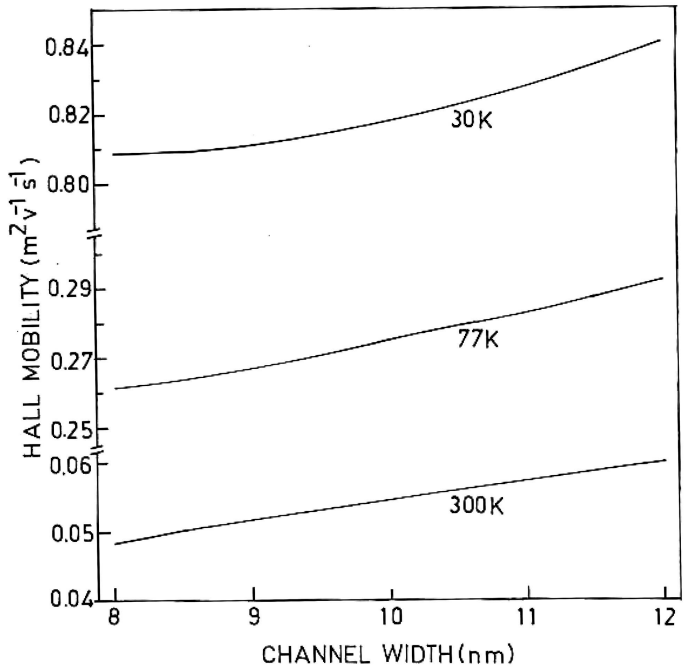

Figure 2. Hall mobility vs. channel width for 30, 77, and 300 K. The other parameter values are the same as in figure 1.

for figure 1. The increase of the mobility with increasing channel width in figure 2 reflects the predominance of lattice scattering which gets weaker as L_z increases [5]. As the channel width changes from 8 to 12 nm, the mobility is found to increase by 23%, 11.5%, and 3.8% for 300, 77, and 30 K, respectively. The progressively lesser

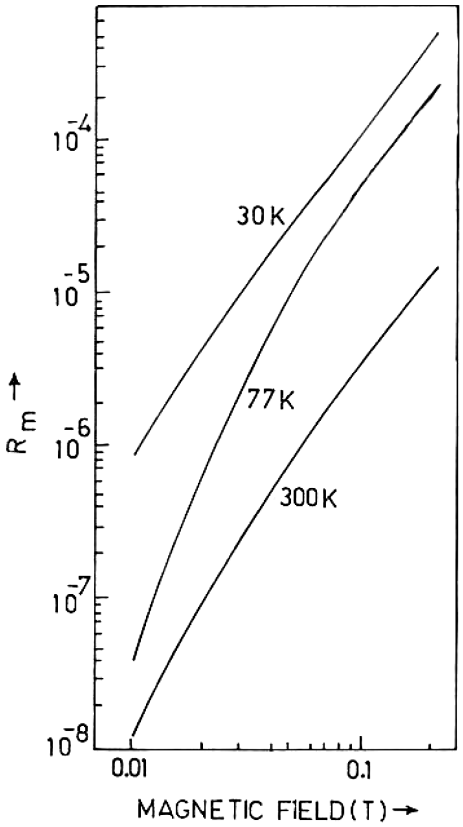

Figure 3. Magnetoresistance coefficient ($R_{\rm m}$) vs. magnetic field for 30, 77, and 300 K. The other parameter values are the same as in figure 1.

effect of L_z on the mobility at lower temperatures is accounted for by the ionized impurity scattering, which gets stronger at lower temperatures and with increasing L_z [5].

The variation of the magnetoresistance coefficient $R_{\rm m}$ with the magnetic field B for temperatures 300, 77, and 30 K is depicted in figure 3. The values of the remaining parameters are the same as those for figure 1. At a fixed temperature, $R_{\rm m}$ is found to increase by several orders of magnitude as B is increased from 0.01 to 0.2 T. The change of $R_{\rm m}$ at 300 and 77 K is more than that at 30 K. For a given magnetic field, $R_{\rm m}$ increases significantly as the temperature drops from 300 to 30 K. The effect is found to be greater at 0.01 T than at 0.2 T.

The magnetoelectronic transport coefficients calculated here depend on the band structure details and on the relative strengths of the relevant scattering mechanisms. So in quantum wells made of materials other than CdSe, the results will be different.

In conclusion, we have presented some new calculations of the Hall mobility and the magnetoresistance coefficient for the two-dimensional electronic transport in CdSe single quantum wells. The remarkable dependence of the calculated results on various parameters, as reported here, suggests that experimental data on

the transport coefficients are needed for a clear understanding of the scattering mechanisms in the CdSe quantum structures. However, to our knowledge, no such experimental data are available as yet in the literature.

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