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Cyclotron resonance of the quasi-two-dimensional electron gas at $Hg_{1-x}Cd_xTe$ grain boundaries

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Abstract. The magnetotransmission of a p-type $Hg_{0.766}Cd_{0.234}Te$ bicrystal containing a single grain boundary with an inversion layer has been investigated in the submillimetre wavelength range. For the first time the cyclotron resonance lines belonging to the various electric subbands of a quasi-two-dimensional carrier system at a grain boundary could be detected. The measured cyclotron masses and the subband densities determined from Shubnikov–de Haas experiments are compared with theoretical predictions and it is found that the data can be explained very well within the framework of a triangular well approximation model which allows for non-parabolic effects.

1. Introduction

It is well known that defects in the region of grain boundaries in various semiconductors can lead to the formation of quasi-two-dimensional (Q2D) carrier systems which are confined in symmetric, V-like potentials. Magnetotransport investigations of inversion layers at grain boundaries in n-Ge [1], p-InSb [2], p-$Hg_{1-x}Mn_xTe$ [3] and p-$Hg_{1-x}Cd_xTe$ [4, 5] have shown that such Q2D systems behave very similarly to those in MIS, hetero- and quantum well structures. In contrast to these artificially produced systems the exact shape of the potential and the nature of the interface states in the grain boundary case is not clear. Measurements of subband densities, cyclotron masses and subband energies which could provide information on the exact shape of the potential well and hence on the space-charge region are therefore of interest.

Investigations of Q2D systems in $Hg_{1-x}Cd_xTe$ are additionally of great interest since for x values of between 0.17 and 0.30 it is a narrow-gap semiconductor with a tunable gap and is therefore an ideal system for study of the effects of non-parabolicity on the properties of the Q2D system. Although numerous experimental [e.g. 6–8] and theoretical [e.g. 9–11] investigations have been made of the properties of quasi-two-dimensional electron gases (Q2DEGs) at HgCdTe surfaces some questions remain open.

In this paper we report the first cyclotron resonance measurements of the Q2DEG adjacent to a grain boundary in a HgCdTe bicrystal. The results of the magneto-optical experiments are compared with data obtained from Shubnikov–de Haas (SdH) experiments and with theoretical models. Furthermore we compare our data with published measurements [6, 7] of Q2D systems in MIS structures and anodically oxidized surfaces of $Hg_{1-x}Cd_xTe$ of comparable x values.

2. Experimental details

The magneto-optical experiments of this paper were performed on a p-type $Hg_{1-x}Cd_xTe$ bicrystal containing a single grain boundary. The bar from which the sample was cut was grown by the seedless travelling heater method (THM) using Te as a solvent. Details of the growth have been previously published [4]. From the as-grown ingot a slab-like sample of dimensions $1 \times 3 \times 4\ mm^3$ was cut by a wire saw which was used for both the transport and optical measurements. To avoid interference effects the sample was wedged. After cutting, the sample was electrochemically polished to produce

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smooth surfaces. For the SdH effect measurements electrical contacts were made to the grain boundary after etching the sample to remove the damaged surface layer.

Hall measurements of a bulk sample cut from a neighbouring part of the ingot yielded a net acceptor concentration $N_A - N_D \simeq 10^{15}$ cm^{-3} [4]. By measuring the energy gap from the energy dependence of the infrared transmission at 77 K we obtained a value of $x = 0.234$, which then gave the low-temperature energy gap as E_g (4.2 K) = 115 meV.

The magneto-optical measurements were performed using an optically pumped molecular gas laser at discrete wavelengths between 47.7 μm and 215.4 μm at a temperature of 4.2 K in magnetic fields of up to 8 T. The measurements were carried out in Faraday configuration, i.e. the magnetic field and the Poynting vector of the electromagnetic radiation were directed perpendicular to the plane of the grain boundary.

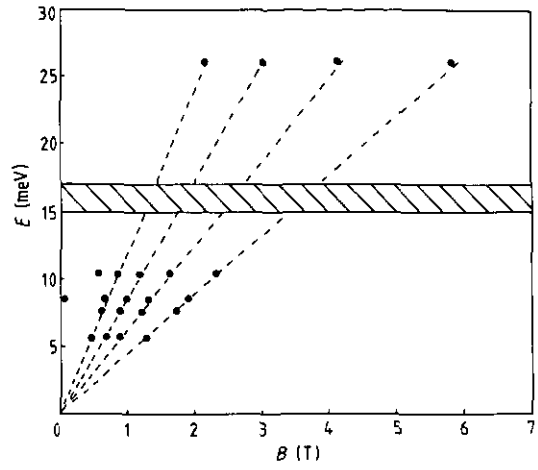

Figure 2. Transition energies plotted against magnetic field. The broken lines are guides to the eye for the cyclotron resonance transitions. The hatched area indicates the HgTe reststrahlen region.

3. Results and discussion

Typical transmission spectra measured at various wavelengths between 118.8 μm and 215.4 μm at $T = 4.2$ K are shown in figure 1. The spectra show several pronounced absorption maxima with the peak at the low-field side of the spectrum much larger than the others. Plotting the photon energies against the resonance field position (figure 2) shows that, excepting a weak resonance which appears only at the wavelengths 118.8 μm and 145.65 μm at fields below the position of the strongest absorption peak, all the extrapolations pass through the origin, i.e. the resonances are the result of cyclotron resonance transitions. The magnetotransmission was not measured for laser wavelengths between 47.7 μm and 118.8 μm since this range is close to the reststrahlen band [7].

An extrapolation of the two data points from the weak low-field resonance to $B = 0$ would yield an energy of about 8.5 meV. This is consistent with an intra-impurity level transition of a shallow acceptor (or the lowest Hg vacancy level) with a binding energy of order 10 meV, similar to the values determined by optical measurements [12-14], but this is not an accurate value as no fitting of the impurity levels was attempted.

The three weak resonances on the high-field side of the spectrum can be identified as cyclotron resonance transitions of the various occupied electric subbands. The corresponding masses were calculated using

$$m_{ci}^* = eB/\omega$$

and are plotted against the photon energy in figure 3. It is well known from theoretical [9, 10, 15] and experimental [6, 7, 16] studies of the effects of a non-parabolic band structure on Q2D electron systems that the cyclotron

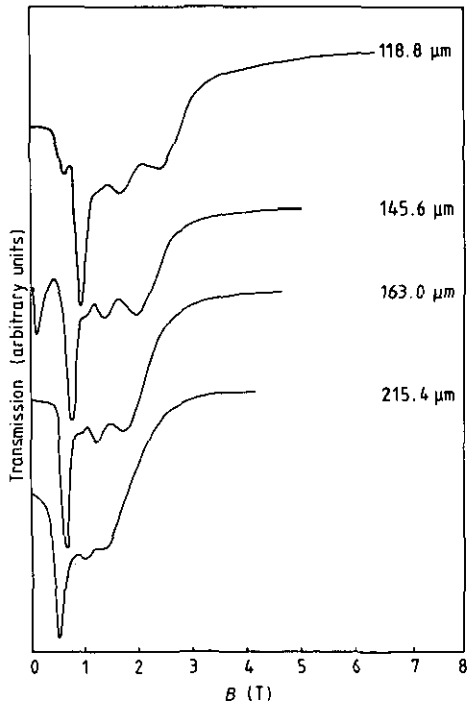

Figure 1. *Transmission spectra versus magnetic field* measured at 4.2 K for various wavelengths.

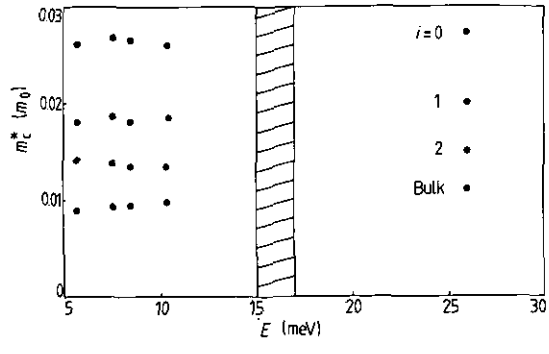

Figure 3. Cyclotron masses of subband and bulk electrons plotted as a function of the photon energy. The hatched area shows the HgTe reststrahlen band. The experimental errors are $\pm 0.002m_0$ for the bulk, $\pm 0.001m_0$ for the $i = 0$ and $i = 1$ subbands and $\pm 0.0015m_0$ for the $i = 2$ subband.

masses of the Q2D carriers are larger than the corresponding band-edge mass and decrease with increasing subband index (except in the case of a simple square-well potential, for which the cyclotron masses of the carriers in different subbands should be equal despite non-parabolicity). Within the experimental errors no dependence of the cyclotron masses on the laser energy was found.

In considering the strongest line in our experimental curves it is worth noting that our spectra are very similar to those measured by Singleton *et al* [7] for anodically oxidized $x = 0.2$ HgCdTe samples. In that case the authors attributed the strong line to bulk electron resonance. Despite the fact that our samples are p-type bulk with a degenerate n-inversion layer at the grain boundary (as is shown by Hall measurements [4]) the large absorption seems to indicate that a bulk effect is again involved. The total absorption corresponds to a sheet density of 4×10^{11} cm^{-2}, which is far higher than could be accommodated in a higher ($i = 3, 4$) subband, but would be consistent with a thin layer of order 4 μm thick and a bulk electron concentration of order 10^{15} cm^{-3}. This would not be detectable in the high-temperature Hall measurements when the bulk holes are thermally ionized as the sheet density in the 1 mm thick samples is 10^{14} cm^{-2}. The energy dependence of the 'bulk' cyclotron mass below the reststrahlen region shows a pronounced slope, and fitting these data with the well known formulae for the conduction band Landau levels of a Kane-like narrow-gap semiconductor [17] with Weiler's parameter set [18] yields values of $E_g = 98 \pm 3$ meV for the gap energy, $m_0^* = (0.0074 \pm 0.0002)m_0$ for the conduction band edge mass and $g_0^* = -115 \pm 5$ for the effective g factor.

Although we have no conclusive evidence we believe that the appearance of a bulk electron cyclotron resonance in the p-type material could result from strong inhomogeneities across the sample. The p-type bars are highly compensated so it could be the case that n-type regions exist. This assumption is supported by a recent measurement in which the submillimetre beam was focused onto a relatively small (about 1 mm diameter) region of the sample and no bulk resonance appeared in the spectrum. The gap energy E_g deduced from the bulk cyclotron resonance position is considerably smaller than that determined from the optical absorption edge, which suggests that the n-type regions would need to have a lower x value than the p-type material, and hence a reduced gap. This is perhaps not unexpected around the region close to a grain boundary. The n-type regions would only need to be a few micrometres thick, as discussed above, so that the infrared transmittance versus photon energy measurement measures the gap energy of the majority of the 1 mm thick sample, while the value obtained from the bulk cyclotron resonance is determined only by the thin n-type areas.

The subband cyclotron masses determined from our cyclotron resonance measurements and shown in figure 3 are considerably smaller than those reported by Kraak *et al* [4] for a sample cut from a part of the ingot adjacent to that from which our sample came. The values obtained by Kraak *et al* were deduced from an analysis of the temperature dependence of the amplitude of the SdH oscillations, giving $m_{c0}^* = 0.037m_0$, $m_{c1}^* = 0.023m_0$ and $m_{c2}^* = 0.017m_0$.

In our earlier work on InSb bicrystals [19] we found that the experimental cyclotron masses and subband carrier densities could be theoretically explained quite well in a triangular-well approximation which included the effect of the non-parabolic band structure. Zawadzki [15] derived the following transcendental equation for the Landau level energies of electrons in a symmetric triangular well

$$(a+b)a^{1/2}b^{1/2} + (b-a)^2 \ln \left| \frac{b^{1/2} - a^{1/2}}{(b-a)^{1/2}} \right| = \left(\frac{E_g}{2m_0^*}\right)^{1/2} 2\pi eF\hbar(i + 1/2) \qquad i = 0, 1, 2 \ldots$$

with

$$a = E - E_{\|} \qquad b = E + E_{\|} + E_g$$

and

$$E = \frac{-E_g}{2} + \sqrt{\left(\frac{E_g}{2}\right)^2 + E_g[\hbar\omega_c(n + 1/2) + s\mu_B g_0 B]}$$

where F is the electric field strength, $E_{\|}$ is related to the non-parabolic bandstructure (see [15] for details), μ_B is the Bohr magneton, ω_c the cyclotron frequency, n the Landau quantum number, i the subband index and s the spin quantum number ($\pm 1/2$). To calculate the cyclotron masses via the equation $m_{ci}^* = \hbar eB/(E_{n+1,i,s} - E_{n,i,s})$ one has to know the position of the Fermi level. This is determined by the filling of the Landau levels, i.e. by the subband densities.

To find the electron densities SdH measurements were performed. A typical curve of the longitudinal magnetoresistance is shown in figure 4. Similar curves have been obtained by Kraak *et al* [4] and Nachtwei *et al* [5] for

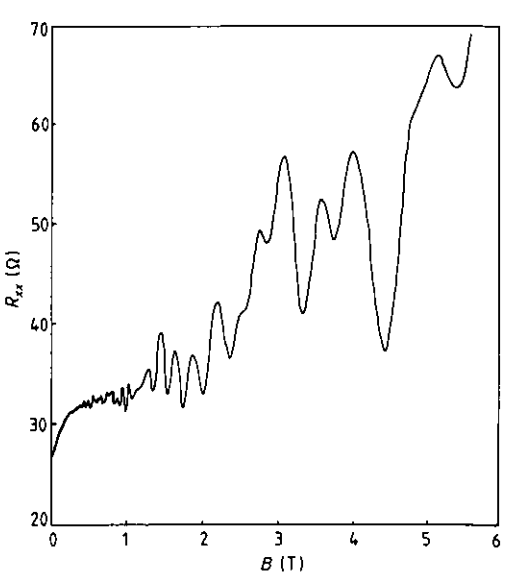

Figure 4. Magnetoresistance R_{xx} versus magnetic field measured at $T = 4.2$ K.

neighbouring HgCdTe bicrystal samples. Detailed investigations in the latter paper using a digital Fourier transform technique have shown that the ρ_{xx} traces are complicated by interfering spin-split levels in addition to the superposition of the sets of Landau levels coming from the different electric subbands. Two sets of oscillation periods were found and it was concluded that an asymmetric potential barrier existed at the grain boundary interface.

A careful analysis of the SdH pattern of figure 4 shows that above 2.1 T the oscillations originate mainly from spin-split levels of the $i = 0$ subband and yield a subband density of $n_{s0} = 6.3 \times 10^{11}$ cm^{-2} whereas in the field range 0.13 T $< B <$ 2.1 T three main periods could be detected which are due to the spin degenerate $i = 0, 1, 2$ with electron densities of

$$n_{s0} = 5.4 \times 10^{11}\ \text{cm}^{-2}$$

$$n_{s1} = 1.7 \times 10^{11}\ \text{cm}^{-2}$$

$$n_{s2} = 0.44 \times 10^{11}\ \text{cm}^{-2}.$$

In principle the two n_{s0} values could indicate the presence of two different subbands. The difference in carrier concentration, however, only amounts to about 17% and is probably due to the redistribution of electrons into the $i = 0$ subband as the higher subbands are emptied. Another explanation could be the existence of a slightly asymmetric double potential well at the grain boundary and consequently of two Q2DEGs as discussed by Nachtwei *et al* [5]. It is interesting to note that, contrary to our experience with InSb bicrystals, where we found comparable values of the total Q2D electron concentration for all samples, HgCdTe bicrystals cut from the same ingot exhibit large differences in their electronic properties.

With the subband carrier densities known the electric field strength F and the position of the Fermi level E_F were adjusted so as to obtain the best fit to the experimental values of the n_{si}. Table 1 shows the best fits which were obtained using a value of $E_g = 115$ meV and $F = 5 \times 10^4$ V cm^{-1}, and $E_F = 125$ meV.

It is clear that the fits obtained for the masses are in good agreement with the experimental data. A variation of the bandgap, and consequently of the band-edge mass m^*_{c0}, has only a small influence on the results. The fits do, however, only give two occupied subbands, which is a reflection of the fact that the simple triangular model does not take account of the band bending, and/or any possible change to an accumulation layer due to the type conversion near to the grain boundary.

Table 1. A comparison of the experimentally determined subband masses and densities with those calculated from the triangular well approximation.

	Experimental values	Theoretical fit
E_F(meV)		125
F(V cm^{-1})		5×10^4
n_{s0}(10^{11} cm^{-2})	5.4	5.3
n_{s1}(10^{11} cm^{-2})	1.7	1.7
n_{s2}(10^{11} cm^{-2})	0.44	0
$m^*_{c0}(m_0)$	0.026	0.024
$m^*_{c1}(m_0)$	0.018	0.019
$m^*_{c2}(m_0)$	0.014	

The excellent agreement between experiment and theory seems somewhat surprising since the potential well has been approximated by a simple triangular one and the calculations are based on a model that, while it takes account of the non-parabolicity of HgCdTe, has been found to overestimate the cyclotron masses for given subband populations in InSb [19]. In cyclotron resonance experiments on gated p-InSb samples Merkt *et al* [16] found that the experimental cyclotron masses lie substantially below the theoretical values, although the subband populations and energies are accurately predicted by the theory. InSb has a relatively large bandgap compared with $x = 0.2$ HgCdTe, so that conduction–valence band mixing does not seem to be the cause of the discrepancy. Cyclotron resonance and SdH measurements by Singleton *et al* [20] of accumulation layers at various anodic oxide films on $x = 0.2$ n-HgCdTe showed a similar behaviour. These measurements, the InSb inversion layer measurements and work on the electric spin-splitting of the subbands in inversion layers on p-type HgCdTe [21] all differ from the present results in that they were carried out on systems with asymmetric confining potentials. In contrast to such asymmetric potentials the effects of the confining electric fields will be minimized in the symmetric potential of the bicrystal.

4. Summary

In this paper we have reported the first successful cyclotron resonance measurements of the Q2DEG adjacent to the grain boundary of a p-type HgCdTe bicrystal. In contrast to our previous experiments on InSb bicrystal samples [19], the cyclotron resonance lines belonging to different occupied electric subbands could be detected. The experimental cyclotron masses and the subband carrier densities determined from the SdH oscillations agree very well with calculations which have been performed in a simple triangular-well approximation. Nevertheless, questions remain concerning the observation of a bulk electron cyclotron resonance in the p-type HgCdTe material, the discrepancy in the gap values determined by infrared transmission and cyclotron resonance measurements and the analysis of the SdH data. These points are the subject of further investigations.

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