Infrared-absorption spectra of acceptors confined in GaAs/$Al_xGa_{1-x}As$ quantum wells in the presence of an external magnetic field

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The infrared-absorption spectra of acceptors confined in the center of GaAs/$Al_xGa_{1-x}As$ quantum wells in the presence of an external magnetic field have been calculated. The calculations are based on a four-band effective-mass theory in which the valence-band mixing as well as the mismatch of the band parameters and the dielectric constants between well and barrier materials have been taken into account. The dipole transition rule is assumed for the infrared absorption. The oscillator strengths of allowed transitions between the acceptor ground states and excited states, corresponding to the transitions *G*, *D*, and *C* in bulk GaAs, are calculated for different well widths in the range 50–200 Å with an external magnetic field up to 10 T. The oscillator strength of these infrared acceptor transitions exhibits a strong polarization dependence.

INTRODUCTION

The infrared absorption of acceptors confined in quantum-well (QW) structures has so far been very rarely studied both experimentally and theoretically. To the best of our knowledge only one preliminary experimental work reported the infrared absorption of acceptors confined in QW structures.[1] Experimentally the infrared absorption between acceptor states in QW's is more difficult to observe than in the bulk case,[2] due to the broadening of absorption lines as well as a small absorption volume in a QW. Theoretically, due to the complicated valence-band structure, it is more difficult to properly calculate the ground as well as the excited acceptor states in the presence of an external magnetic field. Recently we have presented detailed calculations of acceptor energy levels in QW's in the presence of a magnetic field parallel to the growth direction.[3,4] The theoretical calculations are based on an extension of the zero magnetic-field calculations on acceptors in QW's by Pasquarello and co-workers[5–7] to cover the case of an external magnetic field. An obvious advantage of this theory is that it allows one to obtain the acceptor ground states as well as the excited states of any symmetry within the same framework. The impurity states are calculated within a four-band effective-mass theory, in which the valence-band mixing as well as the mismatch of the band parameters and the dielectric constants between the well and barrier materials have been taken into account.

In previous papers[3,4] we have calculated the magnetic-field dependence of the acceptor energy levels in QW's. The transitions between the acceptor ground $1S_{3/2}$ states and the different excited states were deduced in the presence of an external magnetic field. The calculated $1S_{3/2}(\Gamma_6)$-$2S_{3/2}(\Gamma_6)$ transition energies were in excellent agreement with the experimental results for a different magnetic-field strength.[3] The validity of defining g values for different acceptor levels was also discussed.[4] The g factors of the shallow acceptor $1S_{3/2}$ ground states and the $2P_{3/2}$ excited states were obtained for QW's with different well widths.

In this work, we use the energy eigenvalues and wave functions derived from the previous calculations[4] to calculate the infrared-absorption oscillator strength of each transition at various magnetic-field strengths. The splitting of the infrared acceptor transitions, the oscillator strength of each transition, and polarization effects at different magnetic fields have been thoroughly investigated for acceptors confined in the center of QW's with well widths in the range 50–200 Å. In the following, we briefly discuss the calculations of the acceptor levels in QW's, and the oscillator strength formalism. The calculated absorption spectra are then presented, and finally a discussion and a summary are given.

INFRARED ABSORPTION AT NEUTRAL ACCEPTORS

The energy levels (E^m) and wave functions (F^m) of acceptors confined in the center of QW's can be obtained by solving the Schrödinger equation

$$HF^m = E^m F^m \ . \tag{1}$$

In our calculations we only consider the case of a magnetic field parallel to the growth direction of the QW

structures (denoted as the z direction) by defining the vector potential $\mathbf{A}$ as $\mathbf{A}=(\mathbf{B}\times\mathbf{r})/2=(-yB/2,xB/2,0)$. Here B is the magnetic-field strength along the z direction. The detailed acceptor Hamiltonian H which takes into account the magnetic-field effects has been described in our previous papers.[3,4] The acceptor wave functions can be expressed in terms of a four-component envelope function,

$$F^m(\rho,\theta,z)=[F^{m,s}]$$
$$=[F^{m,3/2},F^{m,1/2},F^{m,-1/2},F^{m,-3/2}]\ ,$$

with s running over the spin indices $-\frac{3}{2}$, $-\frac{1}{2}$, $\frac{1}{2}$, and $\frac{3}{2}$. m is the hole angular momentum and is a good quantum number. The envelope function $F^m(\rho,\theta,z)$ is separable in the coordinates ρ and z,

$$F^{m,s}(\rho,\theta,z)=e^{i(m-s)\theta}\sum_n \rho^{|m-s|}\sum_l A_{nl}^{m,s}e^{-\alpha_l\rho}g_n^s(z)\ . \quad (2)$$

Here the function g_n^s is chosen to be the s-spin component of the four-component envelope function g_n, which describes a QW subband state at $k_\parallel=0$. It is important to note that the full Hamiltonian of acceptors in center-doped QW's has the time-reversal symmetry without applying an external magnetic field. Therefore each acceptor state in QW structures is doubly degenerate at zero magnetic field, i.e., states with the same parity (with respect to inversion of the center of the QW) and with angular momenta $+|m|$ and $-|m|$ are degenerate. In order to distinguish between the two $\pm|m|$ states of a doublet, it is useful to consider the reflection operator σ with respect to the $z=0$ plane. The two states with $\pm|m|$ of a doublet can be chosen to have opposite parity with respect to σ.[5] With an external magnetic field, on the other hand, the time-reversal symmetry is broken, and the degeneracy will be lifted. A detailed discussion of the symmetry for different acceptor states at zero magnetic field can be found in Refs. 5 and 7.

The dipole transition rule is assumed for transitions between acceptor states. The oscillator strength of transitions from the ground state to the excited state is given by

$$f_{i0}^{m'm}(\varepsilon)=2m_0(E_i^m-E_0^{m'})/(\hbar^2\gamma_1)|\langle F_0^{m'}|\varepsilon\cdot\mathbf{r}|F_i^m\rangle|^2\ . \quad (3)$$

Here $E_0^{m'}$, $F_0^{m'}$ and E_i^m, F_i^m are the energies and envelope functions of ground and excited states, respectively, ε is the polarization vector of the electromagnetic radiation, and γ_1 is the valence-band Luttinger parameter.

According to Eq. (3) and the acceptor wave function given in Eq. (2), the transition rules for the electromagnetic transitions allow only transitions between acceptor states of opposite parity with respect to inversion. Consequently for the case of x polarization, only transitions between acceptor states with $\Delta m=\pm1$ and of the same parity with respect to the reflection operator σ are allowed. On the other hand, z-polarized transitions occur only between acceptor states with $\Delta m=0$ and of opposite parity with respect to the operator σ.

RESULTS AND DISCUSSION

We present in this section the calculated infrared absorption spectra of acceptors confined in center-doped GaAs/$Al_{0.3}Ga_{0.7}As$ QW's. The Luttinger parameters given in Table I are used in this calculation. The parameters for $Al_xGa_{1-x}As$ are obtained by linear interpolation between GaAs and AlAs. The valence-band discontinuity is taken to be $\Delta V=0.35\times1247\times x$ meV.

The most comprehensive experimental far-infrared (FIR) study of acceptors in bulk GaAs was reported by Kirkman, Stradling, and Lin-Chung,[2] measured by photoconductivity in the presence of an external magnetic field. Several sharp features, labeled as C, D, and G, were observed. The assignment of these features is the following:[2] G line, $1S_{3/2}(\Gamma_8)$-$2P_{3/2}(\Gamma_8)$; D line, $1S_{3/2}(\Gamma_8)$-$2P_{5/2}(\Gamma_8)$; C line, $1S_{3/2}(\Gamma_8)$-$2P_{5/2}(\Gamma_7)$. The D transition is dominating the FIR spectrum. In QW structures, the symmetry is reduced to D_{2d}. The Γ_8-symmetry acceptor state in bulk material will split into two doublet states of Γ_6 and Γ_7 symmetry in center-doped QW's. Therefore the acceptor G, D, and C transitions in bulk GaAs will split in QW structures as follows: For the G transition, $1S_{3/2}(\Gamma_6)$-$2P_{3/2}(\Gamma_6)$, labeled as $G_z^{h\,-3/2}(\pm)$; $1S_{3/2}(\Gamma_6)$-$2P_{3/2}(\Gamma_7)$, labeled as $G_x^{h\,-1/2}(\pm)$; $1S_{3/2}(\Gamma_7)$-$2P_{3/2}(\Gamma_6)$, labeled as $G_x^{l\,-3/2}(\pm)$; $1S_{3/2}(\Gamma_7)$-$2P_{3/2}(\Gamma_7)$, labeled as $G_{z,x}^{l\,-1/2}(\pm)$.

For the $1S_{3/2}$ acceptor states, the Γ_6 and Γ_7 symmetries correspond to the dominating heavy (hh) and light hole (lh) character, respectively. The G_x and G_z notations correspond to transitions with x and z polarization, respectively. Each transition is doubly degenerate at zero magnetic field, for example, $G_z^{h\,-3/2}(\pm)$ corresponds to the transitions $|+\frac{3}{2}\rangle\rightarrow|+\frac{3}{2}\rangle$ and $|-\frac{3}{2}\rangle\rightarrow|-\frac{3}{2}\rangle$, respectively. In the presence of an external magnetic field, these doubly degenerate states split further, which in turn result in the $G_z^{h\,-3/2}(+)$ and $G_z^{h\,-3/2}(-)$ transitions of different energy. In these notations, $G(+)$ and $G(-)$ represent the transitions involving the ground state with the positive and the negative hole angular momentum projected along the magnetic-field direction, respectively. Analogous notations are also applied in the following for the D and C transitions.

For the D transition, $1S_{3/2}(\Gamma_6)$-$2P_{5/2}(\Gamma_7)$, labeled as $D_z^{h\,-3/2}(\pm)$; $1S_{3/2}(\Gamma_7)$-$2P_{5/2}(\Gamma_7)$, labeled as $D_{z,x}^{l\,-1/2}(\pm)$; $1S_{3/2}(\Gamma_6)$-$2P_{5/2}(\Gamma_7)$, labeled as $D_x^{h\,-5/2}(\pm)$; and for the C transition, $1S_{3/2}(\Gamma_6)$-$2P_{5/2}(\Gamma_6)$, labeled as $C_z^{h\,-3/2}(\pm)$; $1S_{3/2}(\Gamma_7)$-$2P_{5/2}(\Gamma_6)$, labeled as $C_x^{l\,-3/2}(\pm)$. The acceptor absorption spectrum in QW structures is accordingly

TABLE I. The Luttinger parameters.

	GaAs	AlAs
γ_1	6.85	3.45
γ_2	2.10	0.68
γ_3	2.90	1.29
ε	12.53	9.80
κ	1.20	0.12
q	0.04	0.03

more complicated than in bulk GaAs. In the following we present the calculated results from the $GaAs/Al_{0.3}Ga_{0.7}As$ QW's with four different well widths, i.e., 50, 100, 150, and 200 Å. For each well size, the acceptor infrared-absorption spectra in the energy range of the *G*, *D*, and *C* transitions are calculated for three different magnetic fields; 0, 5, and 10 T. Both the *x* polarization (σ component) and the *z* polarization (π-component) of the acceptor transitions from the $1S_{3/2}(\Gamma_6)$ hh acceptor ground state or the $1S_{3/2}(\Gamma_7)$ lh acceptor state are calculated. To make the discussion more clear, the results are classified into four groups according to polarization and carrier of the ground states involved in the transitions. The first and the second groups (Figs. 1 and 2) correspond to the *x*- and *z*-polarization transitions with the $1S_{3/2}(\Gamma_6)$ acceptor state as the ground state, respectively. The third and fourth groups (Figs. 3 and 4) correspond to the *x*- and *z*-polarization transitions with the $1S_{3/2}(\Gamma_7)$ acceptor state as the ground state, respectively. A Gaussian broadening is introduced for all transitions with a Gaussian broadening parameter of 0.2 meV. The oscillator strength of each transition in Figs. 1–4 clearly shows the relative absorption strength without considering thermal population effects of the hh $1S_{3/2}(\Gamma_6)$ and lh $1S_{3/2}(\Gamma_7)$ ground states (i.e., the initial states involved in the transitions are taken to have equal occupation). The notations in Figs. 1–4 have the same meaning as discussed above, but only the angular momenta of the final states in absorption are indicated in the notations since the transitions are classified according to the polarization and the initial states of absorption.

Since the hh $1S_{3/2}(\Gamma_6)$ and the lh $1S_{3/2}(\Gamma_7)$ acceptor states split in QW structures, the thermalization factor should be taken into account when comparing the absorption spectra from these two different ground states. Figure 5 shows the energy separation between the

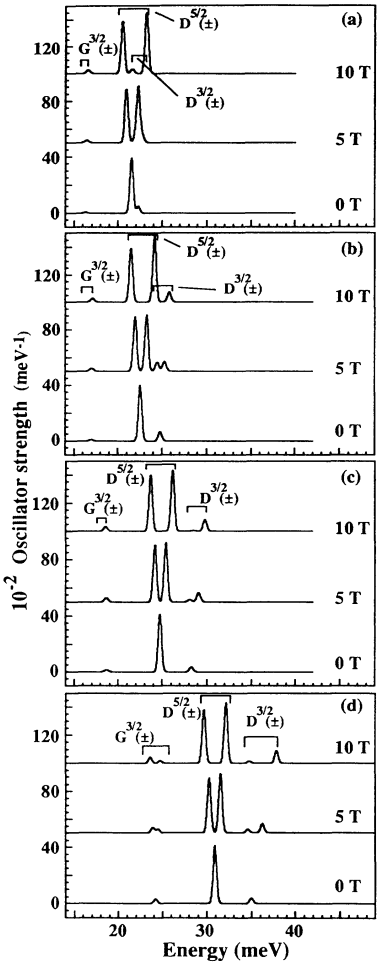

FIG. 1. The oscillator strengths of the *C*, *D*, and *G* absorption lines from the $1S_{3/2}(\Gamma_6)$ hh acceptor ground state in the acceptor spectrum vs the transition energy for *x polarization* in the $GaAs/Al_{0.3}Ga_{0.7}Al$ QW's. The well width is (a) 200 Å, (b) 150 Å, (c) 100 Å, and (d) 50 Å. For each QW width three spectra are shown corresponding to magnetic fields of 0, 5, and 10 T. The spectra at a finite field are offset relative the zero field spectrum for clarity.

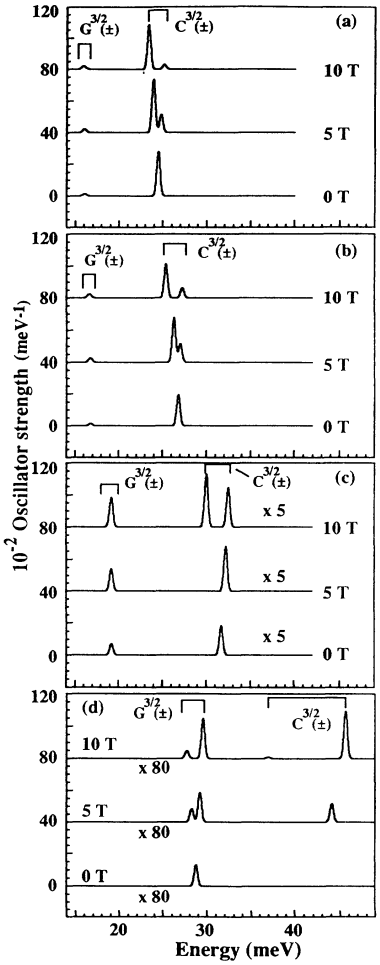

FIG. 2. The oscillator strengths of the *C*, *D*, and *G* absorption lines from the $1S_{3/2}(\Gamma_6)$ hh acceptor ground state in the acceptor spectrum vs the transition energy for *z polarization* in the $GaAs/Al_{0.3}Ga_{0.7}Al$ QW's. The well width is (a) 200 Å, (b) 150 Å, (c) 100 Å, and (d) 50 Å.

$1S_{3/2}(\Gamma_7)$ and the $1S_{3/2}(\Gamma_6)$ acceptor ground states as a function of QW width at zero magnetic field. The ratio of the hole occupancy between the $1S_{3/2}(\Gamma_7)$ and the $1S_{3/2}(\Gamma_6)$ acceptor ground states due to thermalization is also shown in Fig. 5 for three different temperatures. The thermal population of carriers in the $1S_{3/2}(\Gamma_7)$ acceptor states strongly decreases with decreasing well width. At 4.2 K, the absorption strengths of the transitions from the $1S_{3/2}(\Gamma_7)$ ground state is significantly lower than from the $1S_{3/2}(\Gamma_6)$ ground state due to the thermalization effects for narrow QW's. Therefore with decreasing well width resulting in an increase of the energy separation between the $1S_{3/2}(\Gamma_6)$ and the $1S_{3/2}(\Gamma_6)$ acceptor states, the transitions from the $1S_{3/2}(\Gamma_6)$ ground state become increasingly important in the infrared-absorption spectrum. In order to perform an adequate comparison with an experimental infrared-absorption spectrum, we should consider both the oscillator strength (Figs. 1–4) and the thermalization effects (Fig. 5). If we wish to observe the transitions related to the $1S_{3/2}(\Gamma_7)$ ground

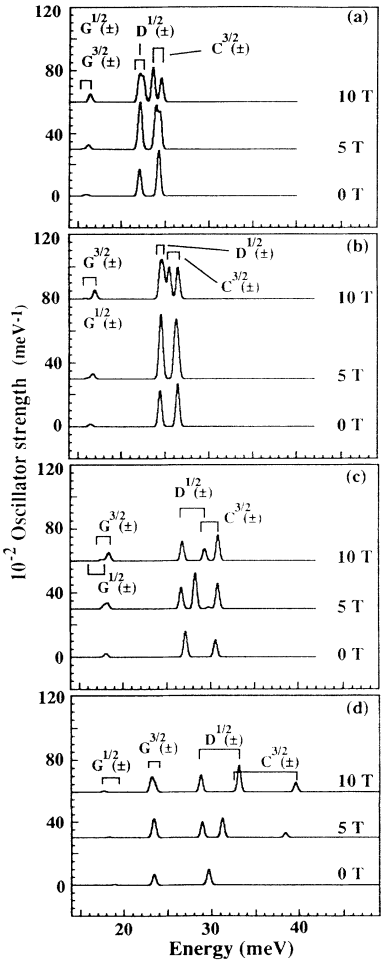

FIG. 3. The oscillator strengths of the *C*, *D*, and *G* absorption lines from the $1S_{3/2}(\Gamma_7)$ lh acceptor ground state in the acceptor spectrum vs the transition energy for *x polarization* in the $GaAs/Al_{0.3}Ga_{0.7}Al$ QW's. The well width is (a) 200 Å, (b) 150 Å, (c) 100 Å, and (d) 50 Å.

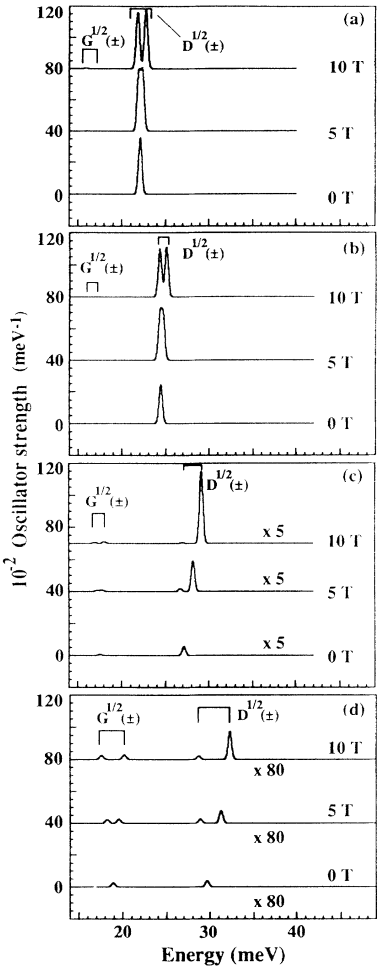

FIG. 4. The oscillator strengths of the *C*, *D*, and *G* absorption lines from the $1S_{3/2}(\Gamma_7)$ lh acceptor ground state in the acceptor spectrum vs the transition energy for *z polarization* in the $GaAs/Al_{0.3}Ga_{0.7}Al$ QW's. The well width is (a) 200 Å, (b) 150 Å, (c) 100 Å, and (d) 50 Å.

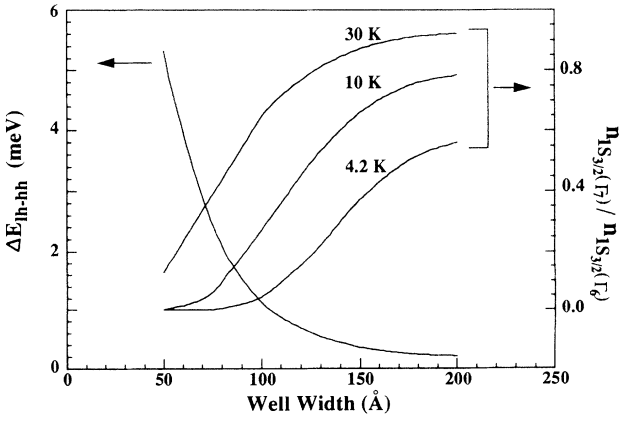

FIG. 5. The energy separations $\Delta E_{lh\text{-}hh}$ (left scale) between the $1S_{3/2}(\Gamma_7)$ and the $1S_{3/2}(\Gamma_6)$ acceptor ground states vs well widths. The ratio of hole population between the $1S_{3/2}(\Gamma_7)$ and $1S_{3/2}(\Gamma_6)$ acceptor ground states due to thermalization (right scale) are also shown for three different temperatures.

TABLE II. The energy separation $\Delta E_{\text{lh-hh}}$ between the $1S_{3/2}(\Gamma_7)$ and the $1S_{3/2}(\Gamma_6)$ acceptor states at zero magnetic field, the g values for the $1S_{3/2}(\Gamma_7)$ and the $1S_{3/2}(\Gamma_6)$ states. The magnetic-field splitting is given by $\pm\mu_B g|J_m|B$, where μ_B (5.7884×10^{-2} meV/T) is the Bohr magneton, and J_m and B are the hole angular momentum and the applied magnetic field, respectively.

QW width (Å)	50	100	150	200
$\Delta E_{\text{lh-hh}}$ (meV)	5.32	1.13	0.36	0.21
g values (hh)	0.757	0.633	0.613	0.605
g values (lh)	−0.230	0.202	0.346	0.432

state, a higher temperature is needed for narrow well widths. Consequently Figs. 1–5 provide general guidance for future experimental investigation of structures of different well widths at different magnetic fields and temperatures.

It should be noted that the thermalization effects between splitting states of the hh $1S_{3/2}(\Gamma_6)$ and the lh $1S_{3/2}(\Gamma_7)$ acceptor states induced by the magnetic field should also be considered. The energy separation between the hh $1S_{3/2}(\Gamma_6)$ and the lh $1S_{3/2}(\Gamma_7)$ acceptor states, as well as g values of these two states[3,4] are shown in Table II for various QW widths and magnetic fields. The magnetic-field splitting at arbitrary field strength can also be obtained from the given g values. Figure 6 shows one example, the x-polarized infrared absorption for a 100-Å-wide QW at 0 and 10 T with various temperatures. At a given temperature the hole populations at different initial acceptor states involved in the absorption are normalized to one at the first ground acceptor state. The bottom spectra in Figs. 6(a) and 6(b) are calculated with equal distribution of holes at the different initial states. The spectra in Fig. 6 clearly demonstrate the temperature dependence of the acceptor infrared absorption.

In general, the D transitions dominate in the FIR absorption spectrum for acceptors confined in QW structures similarly to bulk GaAs. The x-polarization transitions become stronger relative to the z-polarization transitions with decreasing well width. Finally, we would like to point out that some absorption related to other higher excited states besides those discussed above could become relatively strong for the narrow QW's as shown in Fig. 8 in Ref. 7. The transitions shown in Figs. 1–4 correspond to the transitions at the lowest energies with the dominating absorption oscillator strengths without considering hole thermal population effects. The oscillator strengths of the transitions from the $1S_{3/2}(\Gamma_7)$ acceptor ground state become much weaker with decreasing well width, as shown in Figs. 3 and 4. The oscillator strengths of the z-polarized transitions (see Figs. 2 and 4) for 100- and 50-Å-wide QW's have been multiplied by 5 and 80, respectively.

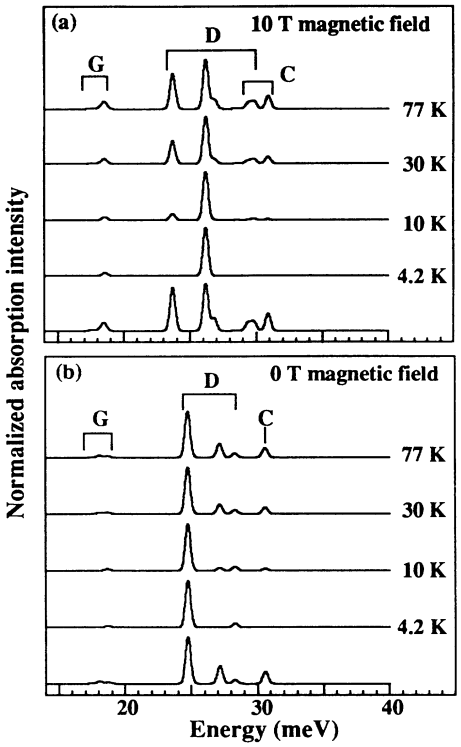

FIG. 6. The temperature dependence of the absorption strength for x *polarization* in a 100-Å-wide GaAs/$Al_{0.3}Ga_{0.7}Al$ QW at 0 and 10 T. The temperature corresponding to each spectrum is labeled at the right side of the spectra. The bottom spectra of (a) and (b) are calculated with equal hole distributions at the different initial states of the transitions.

SUMMARY

The infrared-absorption spectra of acceptors confined in the center of GaAs/$Al_xGa_{1-x}As$ quantum wells in the presence of an external magnetic field have been calculated. The oscillator strengths of allowed transitions between ground acceptor states and excited states, corresponding to the transitions G, D, and C in bulk GaAs, are calculated for different well widths in a range 50–200 Å with an external magnetic field up to 10 T. The oscillator strengths of these infrared acceptor transitions show a strong polarization dependence. To our knowledge, no experimental data relevant for comparison with our calculated results exist to date.

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