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Magneto-optical absorption spectra of periodic superlattices under in-plane magnetic fields

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Abstract. An extensive theoretical study of the magneto-optical absorption spectra of periodic GaAs–(Ga, Al)As superlattices under magnetic fields parallel to the heterostructure interfaces is presented within the framework of the effective-mass approximation. The absorption coefficient associated with interband transitions between valence-hole and conduction-electron magnetic levels is calculated by considering an expansion of the envelope wavefunctions in terms of sine functions and by adopting a parabolic-band model for both electrons and holes. Results for the theoretical magneto-optical interband absorption spectra for varying in-plane magnetic fields compare qualitatively well with various experimental measurements. We present a detailed analysis of the effects of off-diagonal interband transitions involving conduction and valence Landau levels n and n' , respectively, with $\Delta n \neq 0$, and it is unambiguously shown that off-diagonal transitions may introduce significant contributions and extra features in the magneto-optical absorption spectra.

1. Introduction

Man-made heterostructures became an experimentally feasible proposition due to the development of new growth techniques with careful monolayer control and sharp interfaces and have triggered an enormous amount of new physics in the last two decades. Heterostructures of semiconductors with short periods make it possible to observe a variety of quantum effects. The application of a magnetic field parallel to the heterostructure interfaces permits studies of transport of carriers through the superlattice (SL) barriers [1–6].

The optical properties of GaAs–(Ga, Al)As semiconducting periodic SLs have been studied extensively both theoretically and experimentally. In particular, special attention has been given to magneto-optical investigations related to short-period SLs under in-plane (parallel to the interfaces) magnetic fields. Cyclotron resonance experiments in n -doped GaAs–(Ga, Al)As periodic SLs were performed by Duffield *et al* [7], who obtained the intraband absorption spectra. In a recent theoretical work, these experimental results were explained quantitatively by a calculation of the intraband absorption coefficient by de Dios-Leyva and Galindo [8].

Belle *et al* [9] and Maan [10] measured the interband magneto-absorption in GaAs–(Ga, Al)As SLs with a periodicity small compared with the cyclotron radius, under both in-plane and perpendicular magnetic fields. For the case of the in-plane field, they observed

sharp transitions only between the few lowest and flat conduction and valence Landau levels. They argue that, with increasing magnetic field, the highest Landau levels develop a dispersion and become unobservable. Their data were explained with an analysis of the magnetic levels in a Kronig–Penney potential with a magnetic field parallel to the layers, and via a calculation of the joint density of states between conduction and valence Landau magnetic levels. Miura and Sasaki [11] performed magneto-absorption and magneto-luminescence measurements in GaAs–(Ga, Al)As type I and GaAs–AlAs type II short-period SLs in pulsed high magnetic fields of up to 40 T, applied both parallel and perpendicular to the layers, and found well defined oscillatory structures in type I samples for both field directions. They have also calculated the Landau energy levels via a Kronig–Penney SL potential, and claim that the theoretical transition energies were in excellent agreement with the experimental data, except for the ground state where excitonic effects were significant. These last effects were considered in a theoretical work by Dignam and Sipe [12].

In this work, we present an extensive theoretical treatment of the magneto-optical absorption spectra of periodic GaAs–(Ga, Al)As superlattices under in-plane magnetic fields and within the framework of the effective-mass approximation. The motivation for the present investigation is twofold: the above-mentioned experiments on magneto-optical absorption, and that, due to the presence of the SL periodic potential, interband transitions between valence and conduction magnetic levels associated with Landau indices n and n' , with $\Delta n \neq 0$, may occur with a significant contribution to the magneto-optical absorption spectra [13]. Therefore, in order to have an appropriate quantitative understanding of the experimental data, it is certainly necessary to have a realistic calculation of the full magneto-optical $\alpha(\omega)$ interband absorption coefficient. The present work presents a detailed study of a variety of GaAs–(Ga, Al)As SLs. We have first performed calculations for SLs with parameters corresponding to those reported in the experiments of Belle *et al* [9] and of Miura and Sasaki [11] which permits a comparison between our theoretical results and their experimental data. We find that the calculated interband absorption coefficients $\alpha(\omega)$ compare well with both sets of data. We have also considered a GaAs–(Ga, Al)As SL in which the quantum well (QW) width is varied, for fixed in-plane magnetic fields and barrier widths. Results of this calculation show new and interesting evidence for important off-diagonal ($\Delta n \neq 0$) contributions that, in principle, could be observed experimentally.

This work is organized as follows. In the next section, we present our theoretical model framework for the evaluation of the magneto-optical interband absorption coefficient. Theoretical results and discussion are given in section 3 and our conclusions are given in section 4.

2. Theoretical framework

In what follows, we consider a GaAs–(Ga, Al)As periodic superlattice with the growth axis in the y -direction and under a z -direction applied magnetic field parallel to the interfaces. We work in the effective-mass approximation and consider the parabolic band scheme to model both electron and hole levels. The magnetic field is taken as $\mathbf{B} = B\mathbf{z}$ and the gauge for the vector potential is chosen as $\mathbf{A} = -yB\mathbf{x}$. In this case, the effective Hamiltonian for carriers in both the conduction and valence subbands is

$$H = \frac{1}{2m_\alpha^*} \left\{ \left(p_x - \frac{eB}{c} y \right)^2 + p_y^2 + p_x^2 \right\} + V_\alpha(y) \quad (2.1)$$

where m_α^* are the conduction or valence effective masses, e is the proton charge, α refers to either the conduction (c) or the valence (v) magnetic subbands and $V_\alpha(y)$ is the SL

potential with barrier potentials for electrons and holes following the usual 60%–40% rule with respect to the band-gap difference between GaAs and $\text{Ga}_{1-x}\text{Al}_x\text{As}$. This Hamiltonian is translation invariant in the x - and z -directions, and therefore, the wavefunctions may be taken as

$$|n_\alpha \mathbf{k}_\perp\rangle = \frac{e^{ik_x x} e^{ik_z z}}{L_x^{1/2} L_z^{1/2}} \Psi_{n_\alpha, k_x}(y) \quad (2.2)$$

where $\mathbf{k}_\perp = (k_x, k_z)$ and L_x, L_z are the linear dimensions of the sample in the x and z directions, respectively. In equation (2.2), $\Psi_{n_\alpha, k_x}(y)$ satisfies the following one-dimensional Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m_\alpha^*} \frac{d^2}{dy^2} + \frac{1}{2} m_\alpha^* \omega_\alpha^2 (y - y_0)^2 + V_\alpha(y) \right] \Psi_{n_\alpha, k_x}(y) = \varepsilon_{n_\alpha}(k_x) \Psi_{n_\alpha, k_x}(y) \quad (2.3)$$

where $\omega_\alpha = eB/cm_\alpha^*$ is the cyclotron frequency, $y_0 = k_x l_B^2$ is the cyclotron orbit centre position, $l_B = (\hbar c/eB)^{1/2}$ is the cyclotron radius and

$$E_{n_\alpha}(\mathbf{k}_\perp) = \varepsilon_{n_\alpha}(k_x) + \frac{\hbar^2 k_z^2}{2m_\alpha^*} \quad (2.4)$$

is the carrier energy corresponding to the full Hamiltonian (2.1). Energies are measured with the origin at the bottom (top) of the conduction (valence) band of the GaAs bulk (E_g) and with convenient orientations for electrons and holes. Equation (2.3) is solved by expanding $\Psi_{n_\alpha, k_x}(y)$ in terms of sine functions [14], i.e.

$$\Psi_{n_\alpha, k_x}(y) = \sum_m a_m \Phi_m(y) \quad (2.5a)$$

with

$$\Phi_m(y) = \sqrt{\frac{2}{L}} \sin\left(\frac{m\pi y}{L} + \frac{m\pi}{2}\right) \quad m = 1, 2, 3, \dots \quad (2.5b)$$

and with L large enough compared with the superlattice periodicity and with the cyclotron radius of the n_α th calculated Landau magnetic subband.

The interband magneto-optical absorption coefficient is proportional to the transition probability per unit of time involving initial and final states $|i\rangle$ and $|f\rangle$, respectively, and may be obtained via the Fermi golden rule,

$$W(\omega) = \frac{2\pi}{\hbar} \sum_{i,f} |\langle f | H_{\text{int}} | i \rangle|^2 \delta(E_f - E_i - \hbar\omega) \quad (2.6)$$

where $H_{\text{int}} = (eA/m_0c)\varepsilon\Pi$ is the electron–photon interaction Hamiltonian, ε is the polarization vector in the direction of the radiation electric field, $\Pi = (\mathbf{p} + e\mathbf{A}/c)$ is the canonical momentum operator, m_0 is the free-electron mass, A is the amplitude of the photon vector potential and $\hbar\omega$ is the photon energy. In the effective-mass approximation, if one defines

$$T_{n_\nu n_c}(y_0) |\langle \Psi_{n_c k_x} | \Psi_{n_\nu k_x} \rangle|^2 \quad (2.7)$$

and uses the selection rule $\Delta k_\perp = 0$, it is straightforward to obtain the intersubband magneto-optical $\alpha(\omega)$ absorption coefficient [15]

$$\alpha(\omega) \approx \sum_{n_\nu n_c} \sum_{k_z, y_0} T_{n_\nu n_c}(y_0) \delta[E_{n_c}(y_0, k_z) + E_{n_\nu}(y_0, k_z) + E_g - \hbar\omega]. \quad (2.8)$$

The results presented in this work were obtained using the above expressions and convergence was achieved with 300 sine functions in the basis set. Also, in the actual calculation, the above δ -function was replaced by a Lorentzian with a broadening of 8 meV in order to model scattering/resolution effects.

3. Results and discussion

In this section we describe the calculations we have performed using the theoretical framework presented above. Results are first presented for GaAs–(Ga,Al)As SLs with parameters that correspond to the samples in the experiments of Belle *et al* [9] and of Miura and Sasaki [11]. In what follows, the value of the effective mass for electrons at the conduction band was taken as $0.067m_0$, and we have chosen a hole-valence band spherical effective mass of $0.23m_0$, which corresponds to the geometric mean of the light- and heavy-hole effective masses [16].

Results for the interband magneto-optical absorption coefficient $\alpha(\omega)$ for a GaAs–Ga_{0.6}Al_{0.4}As SL, with barrier and QW widths of 1.12 and 3.92 nm, respectively, appropriate for comparison with the experimental measurements of Belle *et al* [9], are presented in figure 1(a). We also present the magnetic Landau conduction and valence subbands corresponding to an in-plane magnetic field of 19 T in figure 1(b). The calculated absorption spectra were evaluated for magnetic fields parallel to the interfaces and corresponded to the values used in the experiments. It is clear from figure 1(b) that the first five, and sharp, peaks in the absorption spectra corresponding to the 19 T magnetic field are associated with $\Delta n = 0$ ‘diagonal’ $n_v \rightarrow n_c$ transitions between essentially flat (non-dispersive) bands with Landau subband numbers running from 0 to 4. Also note that the sixth peak, associated with $n_v = 5 \rightarrow n_c = 5$ transitions, is broadened due to the effect of both valence and conduction subbands becoming dispersive, and that higher-energy peaks are essentially washed out from the spectra also due to dispersive effects, in agreement with experimental data.

In a previous work [13], the 19 T absorption spectrum was calculated using effective masses [9] of $0.64m_0$ and $0.078m_0$ for the valence and conduction bands, respectively. This study took into account transitions involving the six lowest conduction and valence Landau subbands only, with effects of off-diagonal ($\Delta n \neq 0$) $n_v \rightarrow n_c$ transitions associated with Landau subbands found to be significant. In the present calculation, however, the off-diagonal contributions for n_v, n_c up to 5 were found to be less important (see the dotted curves in figure 1(b)) due to the smaller effective masses used in the calculations, which causes a higher number of flat conduction and valence Landau magnetic subbands within the first electron and first hole minibands (in the absence of external fields). We will discuss in more detail the importance of off-diagonal contributions later.

The interband absorption spectra for GaAs–Ga_{0.6}Al_{0.4}As SLs with barriers and widths corresponding to the experimental data of Miura and Sasaki [11] are shown in figure 2, for values of the in-plane magnetic field associated with the experimental measurements. Calculated magneto-optical absorption spectra should be compared with experimental data (cf figure 3), and exhibit essentially the same overall behaviour and trend with decreasing magnetic field. Most noticeable, however, is that, experimentally, for low values of the applied magnetic field, scattering/resolution effects appear to wash out the multiple-peaked spectra shown in the theoretical calculation. Also, one should point out that, in this case, theoretical peaks in the spectra are essentially associated with $\Delta n = 0$ ‘diagonal’ $n_v \rightarrow n_c$ transitions between flat (non-dispersive) Landau subbands.

The theoretical photon energies of some magneto-absorption peaks (cf figures 1(a) and 2) are shown in figure 3 as functions of the magnetic field in the B_{\parallel} configuration. These results are compared with the experimental measurements of Belle *et al* [9] (figure 3(a)) and Miura and Sasaki [11] (figure 3(b)). The qualitative agreement with experiment is apparent, although one must stress that our theoretical calculations do not have any fitting parameter, and we use the standard zero-magnetic field effective mass for the conduction band, and a ‘spherical’ hole-valence band. Also, one should note that the experimental results by Miura

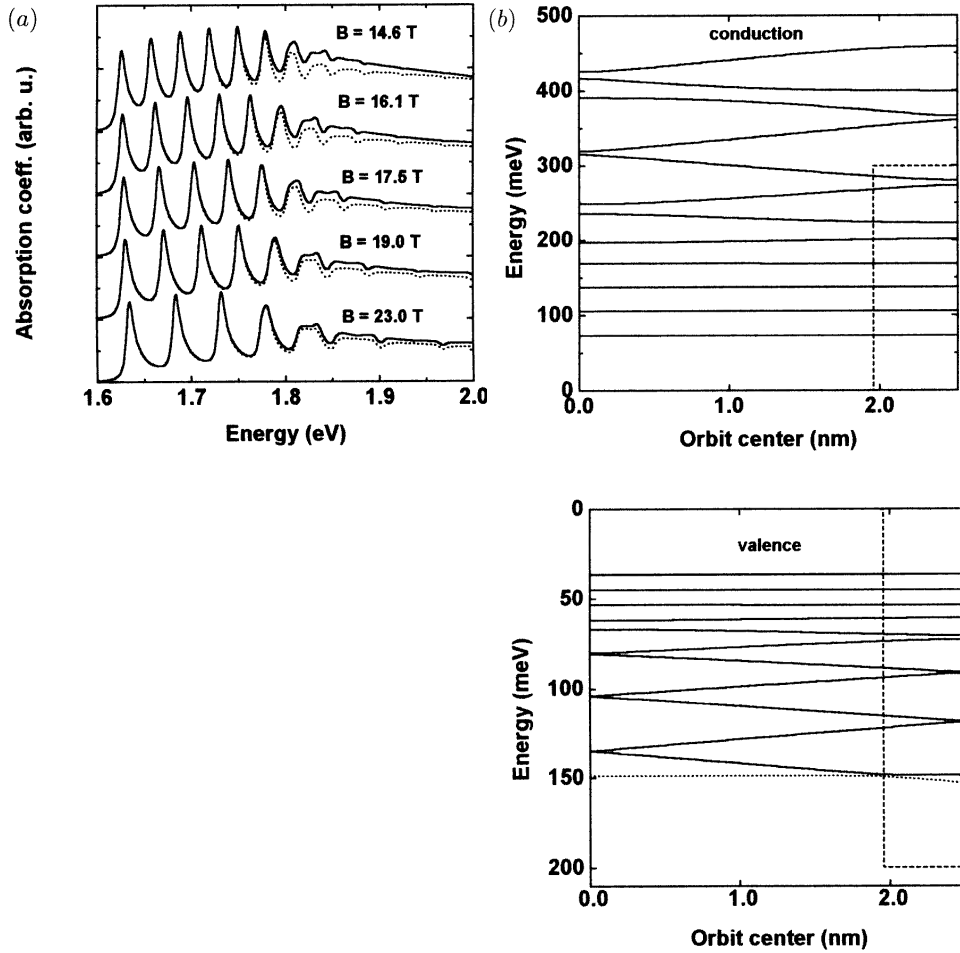


Figure 1. (a) Theoretical magneto-absorption coefficients $\alpha(\omega)$ for a periodic GaAs–Ga_{0.6}Al_{0.4}As superlattice with QW and barrier widths of 3.92 and 1.12 nm, respectively. Results are shown for different in-plane applied magnetic fields. The full curve corresponds to the absorption coefficient with inclusion of all possible transitions (up to Landau subbands $n_v, n_c = 11$), whereas the dotted curve includes only $\Delta n = 0$ transitions; (b) Landau magnetic conduction and valence levels for the case of a magnetic field of 19 T as functions of the cyclotron orbit centre position measured from the QW centre. Broken curves show the SL potential. Note that the $n_v = 10, 11$ subbands exhibit an anticrossing and therefore the $n_v = 11$ subband is shown as dotted, for clarity.

and Sasaki [11] are for an Al concentration of $x = 0.5$, and then, in order to be able to work within the usual one-valley effective-mass approximation, we used a content of 40% of Al in the SL, instead of 50% as for Miura and Sasaki [11]. Therefore, we would not expect a very good agreement with the data of Miura and Sasaki [11] (at this 50% proportion of Al, the importance of transitions involving the X valley will be more important than in the case of the experimental work of Belle *et al* [9]). Of course, a detailed account of the experimental data must involve not only non-parabolicity and valence-band coupling effects but also effects associated with excitons.

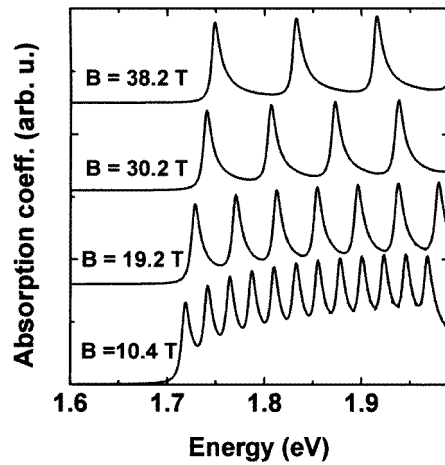


Figure 2. Theoretical magneto-absorption coefficients $\alpha(\omega)$ for a periodic GaAs–Ga_{0.6}Al_{0.4}As superlattice with QW and barrier widths of 1.96 and 1.4 nm, respectively. Results correspond to the absorption coefficient with inclusion of all possible transitions (up to Landau subbands $n_v, n_c = 11$), and are shown for different in-plane applied magnetic fields.

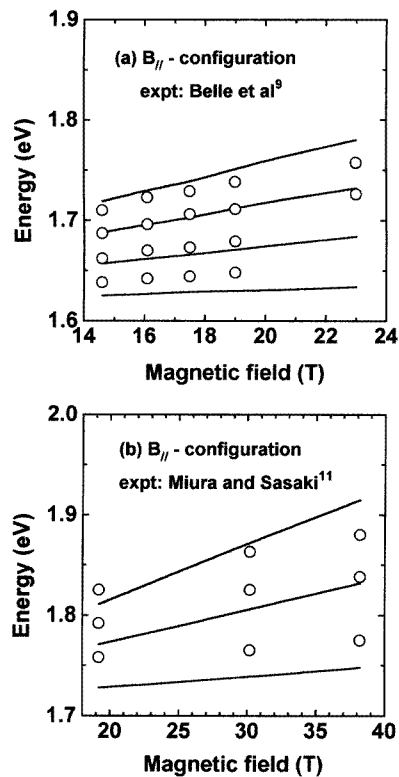


Figure 3. Photon energies of some magneto-absorption peaks as functions of the magnetic field in the B_{\parallel} configuration. Full curves show the theoretical results and open circles denote the experimental values of (a) Belle *et al* [9] and (b) Miura and Sasaki [11].

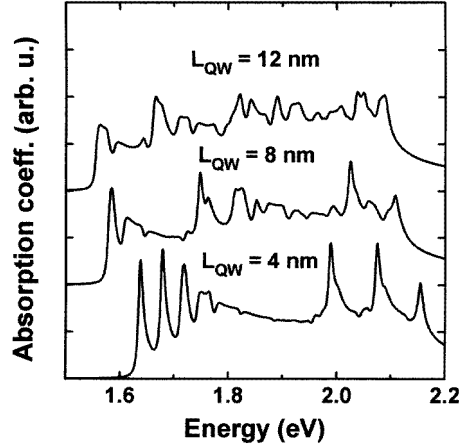


Figure 4. Theoretical magneto-absorption coefficients $\alpha(\omega)$ for a periodic GaAs–Ga_{0.6}Al_{0.4}As superlattice with barrier width of 2 nm. Results are shown for an in-plane applied magnetic field of 20 T, and for different L_{QW} values of the QW width.

In order to further understand the effects of in-plane magnetic fields on the electronic structure and magneto-optical absorption properties of GaAs–(Ga, Al)As SLs, we have performed calculations for a set of three GaAs–Ga_{0.6}Al_{0.4}As SLs, for a 20 T magnetic field, which corresponds to a magnetic length $l_B \approx 6$ nm. For a fixed (Ga, Al)As barrier of width 2 nm, the GaAs QW width L_{QW} was considered as 4, 8 and 12 nm in order to consider the interplay of magnetic length l_B and SL periodicity d (6, 10 and 14 nm, respectively). The magneto-absorption coefficients $\alpha(\omega)$ for these model SLs are shown in figure 4. The corresponding Landau magnetic conduction and valence subbands as functions of the orbit centre position are depicted in figure 5. It is obvious from figure 4 that the absorption coefficients corresponding to the three SLs considered have quite different lineshapes. This may be understood in a quantitative way by an analysis of both the Landau magnetic conduction and valence bands associated with the different SLs and of the transition strengths associated with interband transitions. One should note that these qualitatively different behaviours for the interband absorption coefficients displayed in figure 4 correspond to different regimes which have been studied both experimentally [7] and theoretically [8] in the case of *intraband* transitions for periodic SLs. The interplay of magnetic length and SL periodicity [7, 10] may manifest itself either through a regime associated with dispersive low-lying (cf figure 5(a)) magnetic subbands ($l_B \approx d/2$ or $l_B < d/2$), or through an opposite regime with flat low-lying (cf figure 5(c)) magnetic subbands ($l_B \gg d/2$). It is apparent from figure 5(a) (SL with $d = 14$ nm) that the lowest Landau magnetic conduction and valence subbands present considerable dispersions and many anticrossings leading to quite rich structures in the resulting interband absorption spectrum (see figure 4). For the case of the GaAs–Ga_{0.6}Al_{0.4}As SL with $d = 10$ nm, one finds a behaviour for the magneto-absorption spectrum similar to previous case, except for a sharp peak at 1.58 eV (cf figure 4) due to interband ($n_v = 0 \rightarrow n_c = 0$) transitions associated with flat valence and conduction subbands, as is apparent from figure 5(b). Finally, the absorption spectrum for $d = 6$ nm exhibits a quite different behaviour from those discussed previously. It shows three sharp peaks in the low-energy region clearly associated with $\Delta n = 0$ diagonal $n_v \rightarrow n_c$ transitions between the three lowest-lying flat valence and conduction Landau magnetic subbands (see

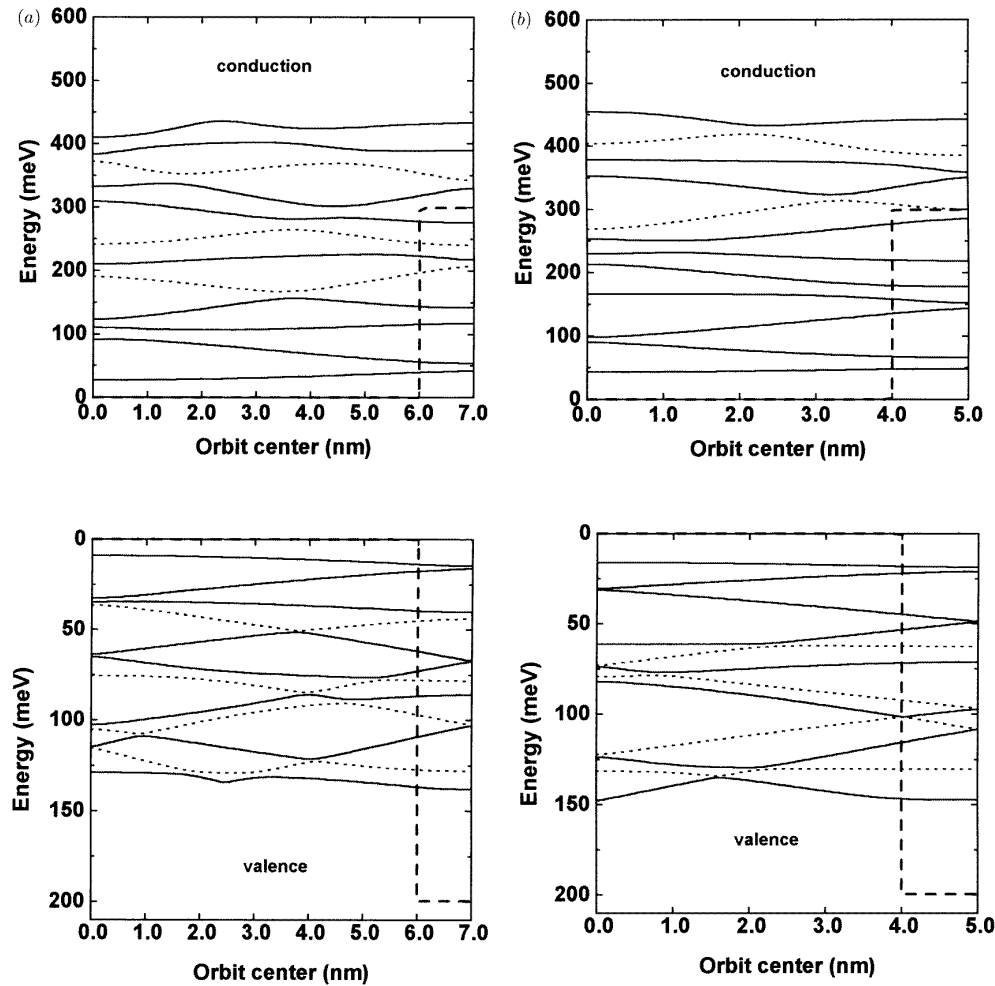


Figure 5. Landau magnetic conduction and valence levels (up to Landau subbands n_v , $n_c = 11$) for a periodic GaAs–Ga_{0.6}Al_{0.4}As superlattice with barrier width of 2 nm and QW width of (a) 12 nm, (b) 8 nm, and (c) 4 nm, as functions of the cyclotron orbit centre position measured from the QW centre. Results are shown for an in-plane applied magnetic field of 20 T. Broken curves show the SL potential. Note that some of the subbands exhibit anticrossings and therefore some subbands are shown as dotted, for clarity.

figure 5(c)), followed by a nearly featureless intermediate region associated with transitions between dispersive Landau subbands, and by three sharp peaks at 1.99, 2.08 and 2.15 eV. The latter peak is clearly associated with the $\Delta n = 0$ diagonal transition between the Landau subbands $n_v = 11$ and $n_c = 11$, whereas the origin of the other two peaks will be detailed below.

To better understand the results presented in figure 4, the interband magneto-optical absorption coefficients for the three model GaAs–Ga_{0.6}Al_{0.4}As SLs are displayed in figure 6 for both the case of the absorption spectrum calculated only taking into account the diagonal $\Delta n = 0$ transitions, and for the absorption coefficient calculated with all contributions (diagonal and $\Delta n \neq 0$ off-diagonal terms). It is apparent that although off-diagonal

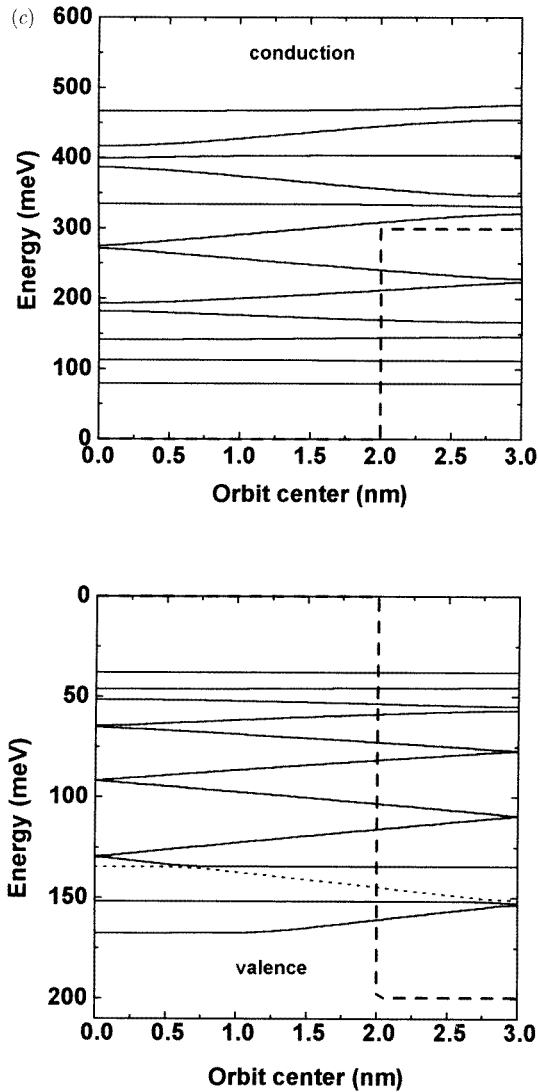


Figure 5. Continued.

contributions from $\Delta n \neq 0$ transitions (associated with $n_v \rightarrow n_c$ transitions between valence and conduction Landau subbands, with $n_v \neq n_c$) are clearly important to be taken into account, they do not change the overall lineshape of the interband absorption spectra for the two SLs considered in figure 6(a) and (b). This is not the case, however, for the absorption spectrum associated with the $d = 6$ nm ($L_{QW} = 4$ nm) GaAs–Ga_{0.6}Al_{0.4}As SL displayed in figure 6(c). Here, the off-diagonal $\Delta n \neq 0$ contributions are such that the absorption presents two sharp lines at 1.99 and 2.08 eV. To understand the origin of these new features, figure 7 displays the most important off-diagonal $\Delta n \neq 0$ contributions for the $L_{QW} = 4$ nm GaAs–Ga_{0.6}Al_{0.4}As SL, and associated with the sharp peaks at 1.99 and 2.08 eV from figure 6(c). It is then clear that the contribution associated with $n_v = 8 \rightarrow n_c = 7$ transitions between valence and conduction Landau subbands are responsible for the extra feature at

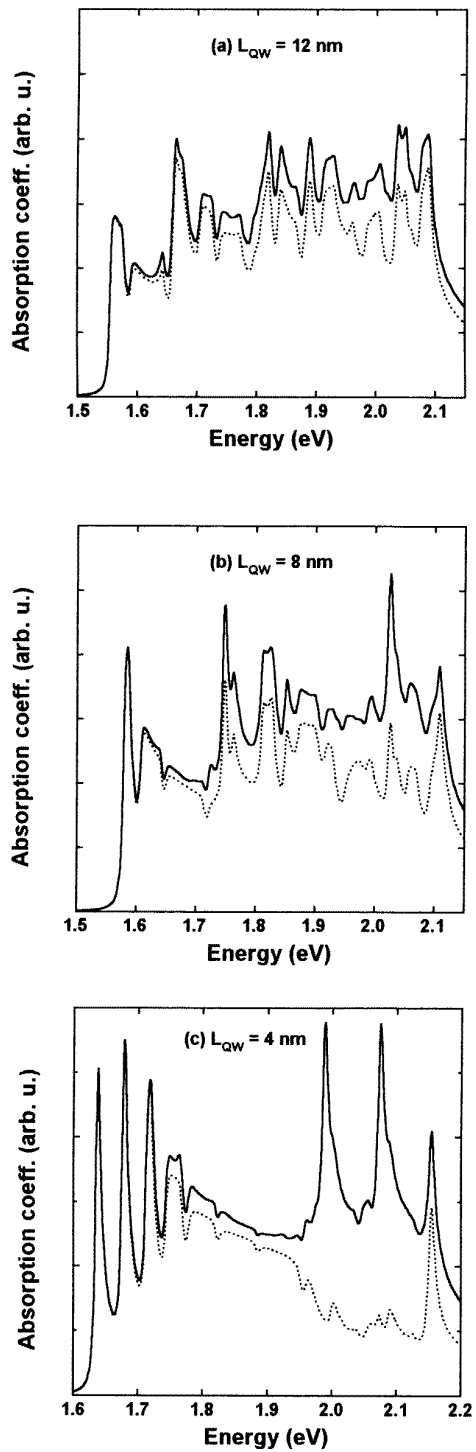


Figure 6. Theoretical magneto-absorption coefficients $\alpha(\omega)$ for a periodic GaAs–Ga_{0.6}Al_{0.4}As superlattice with barrier width of 2 nm. Results are shown for an in-plane applied magnetic field of 20 T, and for values of the QW width, (a) $L_{QW} = 12$ nm, (b) $L_{QW} = 8$ nm and (c) $L_{QW} = 4$ nm. The full curve corresponds to the total absorption coefficient (transitions are considered for Landau subbands up to $n_v, n_c = 11$) whereas the dotted curve displays only the contribution from diagonal $\Delta n = 0$ transitions.

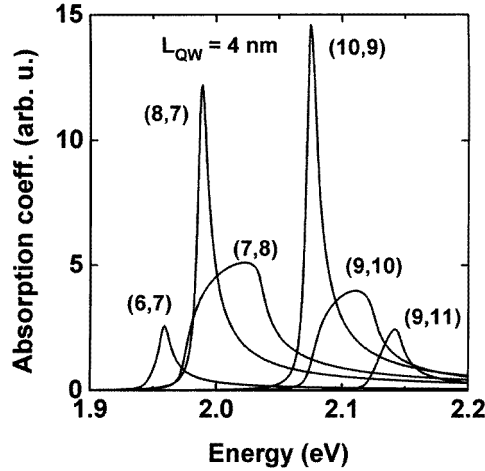


Figure 7. The most important off-diagonal contributions (corresponding to $\Delta n \neq 0$ transitions) to the theoretical magneto-absorption coefficient $\alpha(\omega)$ for a periodic GaAs–Ga_{0.6}Al_{0.4}As superlattice with barrier width of 2 nm. Curves are labelled as (n, n') , and correspond to the interband contribution from the n th Landau valence subband to the n' th Landau conduction subband. Results are shown for an in-plane applied magnetic field of 20 T, and for a value of the QW width $L_{QW} = 4$ nm, and describe main off-diagonal contributions to the peaks at 1.99 and 2.08 eV, from the previous figure 6(c).

1.99 eV, whereas $n_v = 10 \rightarrow n_c = 9$ transitions involving Landau subbands determine the sharp structure at 2.08 eV. Note, however, that the other off-diagonal contributions are also important for the full lineshape depicted in figure 6(c). One should point out that the main off-diagonal contributions to the interband absorption spectrum come from essentially flat $n_v = 8, 10$ valence and flat $n_c = 7, 9$ conduction Landau magnetic subbands, and show unequivocally the importance of considering off-diagonal $n_v \neq n_c$ contributions to the interband absorption coefficient. This effect comes from the large transition strength between high-lying off-diagonal flat-valence to flat-conduction transitions. What is not clear, however, is the physical origin of why only the off-diagonal contribution between high-lying off-diagonal valence and conduction subbands becomes large (and why this does not occur for transitions between off-diagonal low-lying flat subbands). Although Xia and Fan [14] associate the origin of high-lying flat Landau magnetic subbands with electron and hole energy levels in the SL without an applied magnetic field, we believe that a comprehensive understanding of the physics underlying the existence of high-lying flat subbands requires further study. We would like to stress, however, that the presence of the two extra ‘off-diagonal’ sharp peaks in the interband absorption spectrum is unambiguously demonstrated in figures 6(c) and 7 and that these extra features in the spectrum should, in principle, be observed experimentally.

Of course, in a more realistic calculation, the effects associated with excitons, nonparabolicity and valence-band coupling should be taken into account. Excitonic effects were considered by Dignam and Sipe [12], but as pointed out by Belle *et al* [9, 10] their importance is negligible for high-energy exciton-like transitions, as in this case the excitons essentially behave as free electron–hole pairs. Nonparabolicity and valence-band coupling effects, however, are important to be considered if one wants to have a detailed quantitative explanation of the experimental data, although we do believe that consideration of these

effects would not qualitatively modify our predictions on the existence of the two extra 'off-diagonal' sharp peaks in the interband spectrum in figure 6(c).

4. Conclusions

In summary, we have presented a comprehensive theoretical study of the interband magneto-optical absorption spectra of periodic GaAs–Ga_{1-x}Al_xAs SLs under in-plane magnetic fields in the effective-mass approximation. We have considered a sine expansion of the envelope wavefunctions and adopted a parabolic-band model for both electrons and holes, and have studied the interband absorption coefficient $\alpha(\omega)$ associated with transitions between valence-hole and conduction-electron Landau magnetic levels. The theoretical magneto-optical interband absorption spectra for varying in-plane magnetic fields agree qualitatively with various experimental measurements. Moreover, we have presented a detailed study of the importance of off-diagonal $\Delta n \neq 0$ interband transitions involving conduction and valence Landau subbands. Significant off-diagonal contributions and extra peaks in the magneto-optical absorption spectra are shown to appear and should, in principle, be seen experimentally. Furthermore, we have found that extra peaks associated with diagonal transitions may appear at energies corresponding to transitions involving states outside the first electron and hole minibands. This contrasts with the commonly accepted picture [9–11] of the absorption spectra in which, above a certain energy, transitions become unobservable in a parallel magnetic field.

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