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Temperature dependence of the quantized states in a GaAs-$Ga_{1-x}Al_xAs$ superlattice

A. Kangarlu, H. R. Chandrasekhar, M. Chandrasekhar, and Y. M. Kapoor*
Department of Physics and Astronomy, University of Missouri-Columbia, Columbia, Missouri 65211

F. A. Chambers, B. A. Vojak, and J. M. Meese
Amoco Research Center, Amoco Corporation, P. O. Box 400, Naperville, Illinois 60566

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A detailed study of the photoreflectance spectra of a GaAs-$Al_{0.3}Ga_{0.7}As$ superlattice as a function of temperature has revealed the temperature coefficients of the quantum-well transitions associated with the direct Γ conduction band (CB) of GaAs and the staggered transitions from the X-CB of $Al_xGa_{1-x}As$ to the valence band of GaAs. The data have been fitted to Varshni's equation. We have also observed the evolution of the excitonic transitions, especially for lower quantized states, as the temperature is decreased yielding the binding energies.

Modulation spectroscopy, particularly the contactless method of photoreflectance (PR),[1-3] is shown in a very powerful technique to study a large number of quantized states in a multiple-quantum-well (MQW) structure. Considerable discussion on the line shapes of the PR spectra and their changes with temperature has led to the belief that the spectra are excitonic at low temperatures and band to band at temperatures above 250 K.[4,5] A careful analysis of the PR and the photoreflectance excitation (PRE) spectra has led[6,7] to the identification of the 1*s* excitonic state of *Cm*-*Hn* and *Cm*-*Ln* transitions for $m=n=1$. The above notation denotes transitions from the *m*th conduction-band state (C) to the *n*th heavy- (H) or light- (L) hole band state.

We have performed a detailed study of the temperature evolution of the line shapes of PR transitions in a GaAs-$Al_{0.3}Ga_{0.7}As$ MQW with the well width L_z of 260 Å. This study has enabled us to observe a gradual sharpening and the emergence of the 1*s*-excitonic peak from the broad continuum transition as the temperature is lowered for $m(=n)=1$ to 3. The exciton binding energies are determined from this data (Tables I and II). For higher transitions we could not observe this effect because of their large linewidths. We have also observed peaks from transitions originating in the X-conduction band (X-CB) in $Al_xGa_{1-x}As$ across the heterointerface. Due to the band alignment between GaAs and $Al_xGa_{1-x}As$, it turns out that the X-CB in $Al_xGa_{1-x}As$ has its energy lower than that of GaAs. We have performed a calculation of the energy positions of both the Γ and X related transitions and find excellent agreement between the results and experiment. The temperature dependence of the energies of the transitions are fit to the Varshni's equation[8,9] to obtain the coefficients α and β. We find that two sets of α and β can be used to fit the data. The first set of values is very close to the corresponding values for bulk GaAs. We do not see any dependence in the values of α and β with different m (or n).

The samples were grown by molecular-beam epitaxy. The well and barrier widths were estimated from growth parameters. The aluminum mole fraction was deduced from the PL and PRE spectra of a reference $Al_xGa_{1-x}As$ sample grown under identical conditions. The experimental setup is similar to that described in the literature. A variable-temperature cryostat was used.

Figures 1 and 2 show the PR spectrum of the MQW sample at different temperatures. The temperature dependence of various transitions is shown in Fig. 3. The identification of the transitions is also shown in Fig. 3. The numbers with arrows in Figs. 1 and 2 correspond to this identification. The solid and dotted lines passing through the data in Fig. 3 are fitted to the Varshni's equation

$$E(T)=E(T=0)-\alpha T^2/(\beta+T) , \qquad (1)$$

where $E(T)$ is the energy at temperature T.

Figure 1 displays transitions derived from the Γ conduc-

TABLE I. Energies of MQW transitions (in eV) as a function of temperature.

	Temperature (K) 300	250	200	150	125	80
*C*1-*H*1 (ex)	1.424	1.441	1.466	1.488	1.497	1.512
*C*1-*H*1	1.435	1.454	1.476	1.500	1.509	1.524
*C*2-*H*2 (ex)	1.446	1.465	1.488	1.510	1.520	1.534
*C*2-*H*2	1.455	1.472	1.494	1.516	1.524	1.538
*C*3-*H*3 (ex)	⋯	⋯	1.525	1.548	1.556	1.570
*C*3-*H*3	1.490	1.506	1.532	1.554	1.564	1.578
*C*4-*H*4 (ex)	⋯	⋯	1.578	1.599	1.607	1.621
*C*4-*H*4	1.541	1.565	1.587	1.608	1.617	1.631

TABLE II. Binding energies of several MQW transitions for $L_z=260$ Å.

Transition	Binding energy (meV)
*C*1-*H*1	11.8±0.4
*C*2-*H*2	6.0±0.8
*C*3-*H*3	7.3±0.5
*C*4-*H*4	9.5±0.3

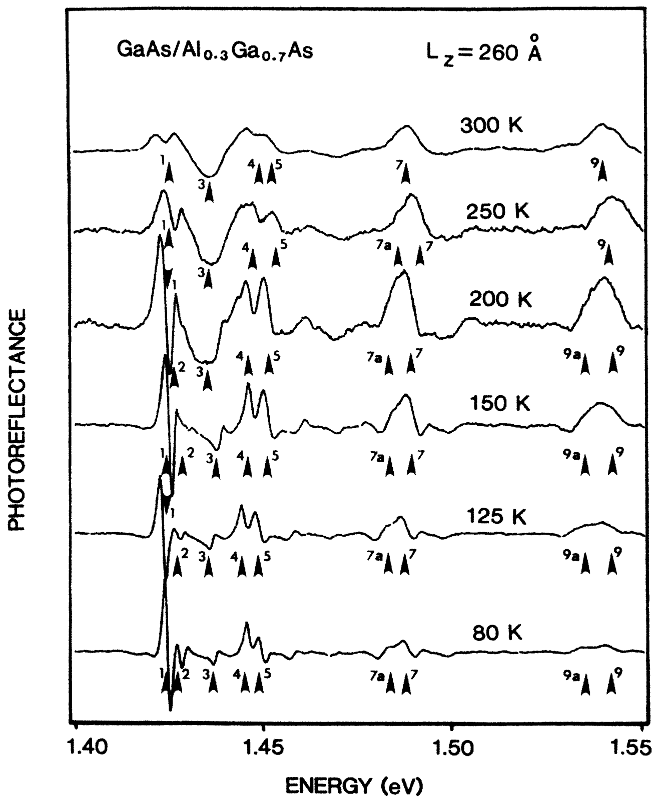

FIG. 1. The photoreflectance spectra of a GaAs/$Al_{0.3}Ga_{0.7}As$ multiple quantum well at different temperatures. Notice that the energy scale corresponds to the spectrum at 300 K. Other spectra have been shifted to align peak 1. The numbers with arrows correspond to transitions derived from the Γ-CB as described in the text. The zero of the PR spectra correspond to the flat part of the reflectivity on the low-energy side.

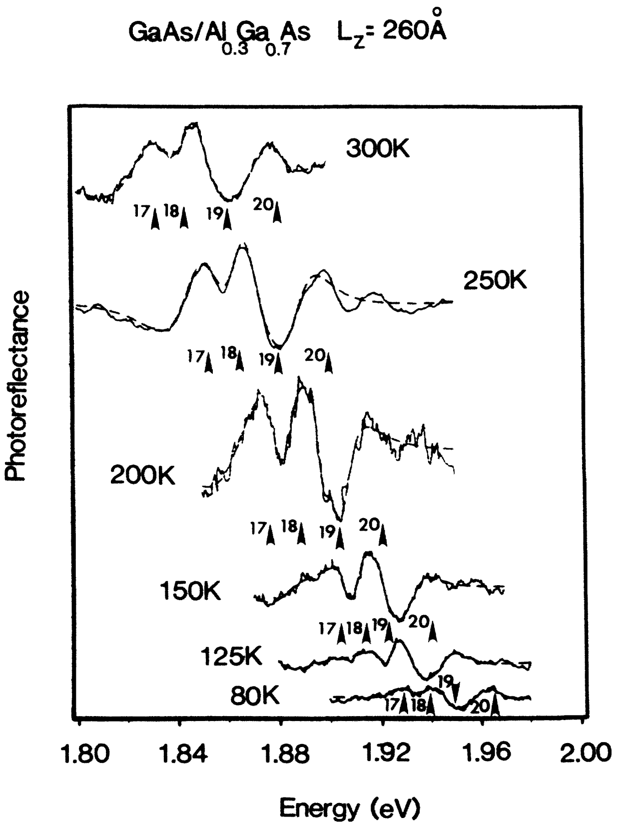

FIG. 2. PR spectra for staggered transitions from the X-CB of $Al_{0.3}Ga_{0.7}As$ (barrier) to the valence band of GaAs (well).

tion band to the heavy- and light-hole valence bands. The energy scale corresponds to the spectrum at 300 K. Other spectra have been shifted to align peak 1. As the temperature is decreased the relative intensities of transitions corresponding to higher m (and n) decrease. This is consistent with the expected decrease in the population of these states as the temperature is lowered. The peaks, in particular for $m=1$ to 3, also sharpen up considerably. The most dramatic change occurs for $C1$-$H1$ transition. At 300 K there is a broad and intense peak at 1.435 eV (denoted by 3) with a weak shoulder (denoted by 1) at a lower energy by about 11 meV. As the temperature is lowered, this shoulder gains intensity at the expense of peak 3. At 200 K, it is as intense as peak 3. For temperatures 150 K and below peak 3 is very much weaker compared to 1. We identify peaks 1 and 3 as the 1S exciton and the continuum (band to band) transitions of $C1$-$H1$, respectively. The separation between them remains constant with temperature. The peaks labeled 4 and 5 in Fig. 1 are due to the $C2$-$H2$ transitions. One can see the changes in relative intensities between these peaks as well. Above 200 K, 4 is weaker than 5 and the reverse is true for lower temperatures. The peak denoted by 7 corresponds to $C3$-$H3$. In this case, a shoulder at lower energy can be easily seen for temperatures below 150 K. At 80 K the peak 7a is as strong as 7. The peak denoted by 9 corresponding to $C4$-$H4$ shows signs of a doubled structure below 125 K. Tables I and II show the peak energies and the exciton binding energies deduced from the data.

Figure 2 shows the spectra associated with the X-CB. The solid curves correspond to the data and the dotted curves are from a fit to the theoretical function[10]

$$\frac{\Delta R}{R}=\mathrm{Re}\left[\sum_{j=1}^{p} C_j e^{i\theta_j}(E-E_j+i\Gamma_j)^{-m_j}\right] , \qquad (2)$$

where ρ is the number of peaks, E is the photon energy, C_j, θ_j, E_j, and Γ_j are the amplitude, phase, energy, and broadening parameters for the jth peak, and m_j is a parameter that depends on the type of critical point and the order of the derivative. We used $m_j=2.5$. Due to the large broadening of these peaks we do not think that we can distinguish between excitonic and band-to-band transitions. The Kronig-Penney-type calculation[11] to evaluate the confinement energies in the X-CB was carried out with the appropriate band parameters. The confinement energies for the first four levels in the X-CB were 1.5, 5.9, 13.3, and 23.4 meV, respectively. The same for the heavy-hole VB were 1.4, 5.4, 12.2, and 21.6 meV, respectively. The energies for peaks 17–20 were obtained by adding the CB and VB confinement energies to 1.839 eV, which is the energy of the X-CB of $Al_{0.3}Ga_{0.7}As$ from the VB of GaAs. Using a conduction- to valence-band offset ratio of 70:30, the energy positions were computed for these transitions.[12] It should be noted that the possibility of these transitions originating from the X band of the well material to its valence band was considered. The observed peaks appear ~40–60 meV lower in energy than expected. These peaks are too high in energy (20–40 meV) to be due to the barrier material.

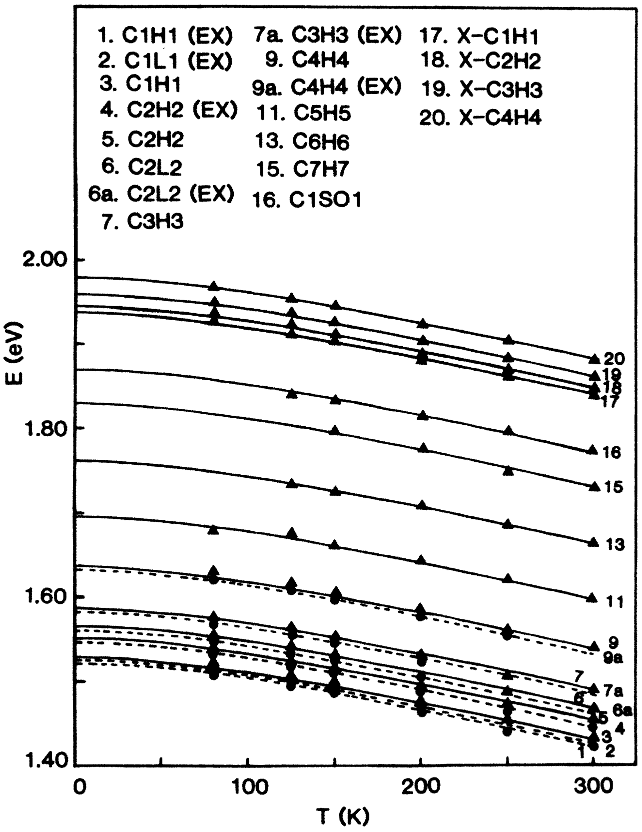

FIG. 3. Temperature dependence of the MQW transitions. The symbols denote the experimental data and the curves are from a fit to Eq. (1) in the text. The dashed curves are from the 1s excitonic transitions and the solid curves are for the band-to-band (continuum) transitions.

The solid and dotted lines passing through the data in Fig. 3 are from a fit to Eq. (1) with values of $\alpha=(5.40\pm0.2)\times10^{-4}$ eV/K and $\beta=204$ K for all the Γ-band derived transitions. The peaks 17–20 had the best fit values of $\alpha=(5.33\pm0.2)\times10^{-4}$ eV/K and $\beta=204$ K. These values are identical to the corresponding coefficients[8,9] for the Γ band of bulk GaAs. We found that all the data taken together can also be reasonably fit by a choice of $\alpha=(4.52)\times10^{-4}$ eV/K and $\beta=108$ K. In that sense α and β are not unique but only represent parameters to describe the temperature dependence. Any relation of β to the Debye temperature of GaAs as originally suggested by Varshni[8] seems inappropriate. Neither of the two values of β are large enough to approach the Debye temperature. The quantum confinement of electrons in the MQW structures has no measurable effect on the temperature behavior of the energy levels which track the band extrema of the well material faithfully. This is in contrast to the pressure dependence of the MQW transitions, where we have shown that the pressure coefficients decrease with increasing confinement (or decreasing well width).[12,13]

There have been several calculations[14,15] of the exciton binding energies. It has been shown that the mixing between heavy- and light-hole subbands away from the zone center can lead to regions of negative mass and can result in sharp peaks in the joint density of states. These mixing effects can lead to larger binding energies for some transitions.[15] The relatively larger binding energies for $C3$-$H3$ and $C4$-$H4$ compared to $C2$-$H2$ are probably due to this effect. A detailed calculation is required to test this point.

In conclusion, we have deduced the exciton binding energies of Cm-Hn transitions and the temperature coefficients of the MQW transitions by a careful study of the PR data. We have also investigated these transitions as a function of hydrostatic pressure.[13] The results will be published elsewhere.

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[*] Permanent address: Department of Natural Sciences and Mathematics, Lincoln University, Jefferson City, MO 65101.

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