Donor-photoluminescence line shapes from GaAs-(Ga,Al)As quantum wells

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The $D^\circ-h$ impurity-related photoluminescence spectra of confined donors in GaAs-(Ga,Al)As quantum wells is theoretically investigated within the effective-mass approximation. The impurity wave functions and binding energies are evaluated via a variational procedure. Calculations are performed for different well widths, temperatures, and impurity doping profiles. Typical $D^\circ-h$ theoretical photoluminescence line shapes show peaked structures corresponding to on-center and on-edge donors in good agreement with experimental results.

The study of impurity states in quantum wells (QW's) was introduced by Bastard[1] who investigated some of the properties of hydrogenic impurities in infinite-barrier QW's. Due to the potential device applications of quantum wells, quantum-well wires, and semiconducting heterostructures in general,[2] the understanding of the nature of impurity states associated with such systems is a subject of considerable technological and scientific relevance. In the past few years, several experimental and theoretical works[3–9] have been devoted to the subject of impurity states in low-dimensional systems and, in particular, to the properties of shallow donors and acceptors in GaAs-(Ga,Al)As QW's.

A recent work[8] on acceptors in GaAs-(Ga,Al)As QW's demonstrated the importance of a proper calculation of the electron→acceptor-band photoluminescence *line shape* when comparing experiment with theoretical results. This has motivated us to do the same study with respect to confined donors in QW's. In this work, therefore, we present a theoretical study of the photoluminescence spectra associated with transitions between the donor-impurity band and the first valence subband ($D^\circ-h$ features) in a GaAs-(Ga,Al)As QW and compare our results with a recent photoluminescence study[5] of confined donors in GaAs-(Ga,Al)As QW's.

We consider a single GaAs-(Ga,Al)As QW of width L with an $N_d(z_i)$ distribution of donor-hydrogenic impurities in which electrons in the donor or in the conduction bands recombine with holes in the valence band. We are concerned with the line shape of the recombination associated with electrons in the donor band. The photoluminescence spectrum associated with the donor band $\rightarrow n=1$ valence-subband transitions is given by[7–9]

$$L(\omega)=(1/L)\int_{-L/2}^{L/2} dz_i[1-\exp(-\beta E_i)]N_d(z_i) \times W_L(z_i,\omega)f(\epsilon_{k_\perp}) , \quad (1)$$

where $f(\epsilon_{k_\perp})=1/\{1+\exp[\beta(\hbar\omega-E_{cv}+E_i-E_F)]\}$ is the Fermi distribution ($\beta=1/k_BT$) for the valence-subband-hole gas, $E_i=E(L,z_i)$ is the binding energy[6] of the donor impurity at the position z_i, and $E_F\simeq 1$ meV is the quasi-Fermi-energy level of the hole-gas in the steady-state quasiequilibrium.[9] The factor $[1-\exp(-\beta E_i)]$ takes into account the thermal ionization of the donors. In the above expression

$$E_{cv}=E_g+E_{n=1}^c+E_{n=1}^v , \quad (2)$$

$$E_g(\text{eV})=1.519-\frac{5.405\times10^{-4}T^2}{T+204} \quad (3)$$

is the temperature-dependent[10] bulk GaAs gap and $E_{n=1}^c$ ($E_{n=1}^v$) is the bottom (top) of the first conduction (valence) subband. For a GaAs-(Ga,Al)As QW of width L, the transition probability per unit time for valence-to-donor transitions is given by[7]

$$W_L(z_i,\omega)=W_0\frac{1}{2}\left[\frac{a_0^*}{a_0}\right]^2\left[\frac{m_v^*}{m_0}\right](N_b^2a_0^*)\frac{N^2J^2}{a_0^{*3}}\bigg|_{k_\perp(z_i,\omega)} \times Y[\hbar\omega-E_{cv}+E(L,z_i)] , \quad (4)$$

where a_0 is the Bohr radius, m_0 is the free-electron mass, $a_0^*=\hbar^2\epsilon_0/(m_c^*e^2)$ is the effective Bohr radius associated to the donor impurity, $Y(x)$ is the step function, $N=(1/\langle\Psi|\Psi\rangle)^{1/2}$ is the normalization factor for the donor variational[6] wave function, and N_b is the normalization factor for the wave function associated to the first valence subband. Also, we have

$$k_\perp(z_i,\omega)=\{2m_v^*[\hbar\omega-E_{cv}+E(L,z_i)]/\hbar^2\}^{1/2} , \quad (5)$$

$$W_0=\frac{4m_0}{\hbar^3}a_0^2|C|^2|\mathbf{e}\cdot\mathbf{P}_{fi}|^2 , \quad (6)$$

in which $\mathbf{P}_{fi}$ is a matrix element,[7] $\mathbf{e}$ is the polarization vector in the direction of the electric field of the radiation, $\mathbf{p}$ is the momentum operator, and C is a prefactor which contains the photon vector potential. The expression for $J=J(z_i,\lambda,k_\perp(z_i,\omega))$ in Eq. (4), where λ is the

donor wave function variational parameter, is given in Ref. 7. Results in this work for the photoluminescence line shape are given in units of

$$\mathcal{W}_0=(L/a_0^*)W_0 \ . \tag{7}$$

We neglect the coupling between the top four valence bands[11] and consider a spherical heavy-hole effective mass $m_v^* \simeq 0.30 m_0$ which gives a bulk value[12] of 26 meV for the effective Rydberg $R_0^* = m_v^* e^4/(2\hbar^2\epsilon_0^2)$. Also, although the effective masses $m_{v,c}^*$ and the dielectric constant vary across the interfaces[13] we assume the values of $m_{v,c}^*$ and of the dielectric constant in GaAs for all regions of the heterostructure. Finally, we choose the band-gap discontinuity in the GaAs-(Ga,Al)As heterostructure as distributed about 40% on the valence band and 60% on the conduction band with the total band-gap difference ΔE_g between GaAs and $Ga_{1-x}Al_xAs$, given[10] as a function of the Al concentration as ΔE_g (eV) $=1.247x$.

The QW doping profiles used in our photoluminescence-line-shape calculations and appropriate for comparison with the experimental work by Liu *et al.*[5] are edge $\frac{1}{3}$ doped, center $\frac{1}{3}$ doped, and homogeneously doped inside the QW. The donor envelope wave functions and binding energies are obtained within an effective-mass variational procedure outlined in previous work;[6] calculations were done for GaAs-(Ga,Al)As QW's with $x=0.3$ concentration of Al and widths of $L=80$, 140, and 210 Å which correspond to the QW characteristics in the study by Liu *et al.*[5]

The theoretical temperature dependence ($T=5$ and 30 K) of the $D^\circ-h$ photoluminescence spectra is shown in Fig. 1 for an $L=210$ Å center-$\frac{1}{3}$-doped GaAs-$Ga_{0.7}Al_{0.3}As$ QW as compared with the experimental results by Liu *et al.*[5] The onsets of the $D^\circ-h$ photoluminescence spectra correspond to the onset of transitions from on-center donors to the valence subband. Of course, the theoretical decrease with the temperature in the $D^\circ-h$ photoluminescence intensity is due to thermal ionization of the donors. Also, notice that there is a 2-meV shift in the photoluminescence spectra due to temperature effects [see Fig. 1 and Eqs. (2) and (3)]. This is absent from the experimental results[5] at $T=30$ K due to an artificial shift[14] of the experimental data in order that the ground-state heavy-hole exciton peak would have the same energy position. The $T=5$ K donor-related theoretical peak in the photoluminescence spectrum at 1522 meV (as $E_{cv}=1531$ meV, this peak would correspond to a donor "binding energy" of 9 meV) correlates very well with feature (iv) of the $T=5$ K experimental result of Liu *et al.*[5] [although in their Fig. 2(a) feature (iv)

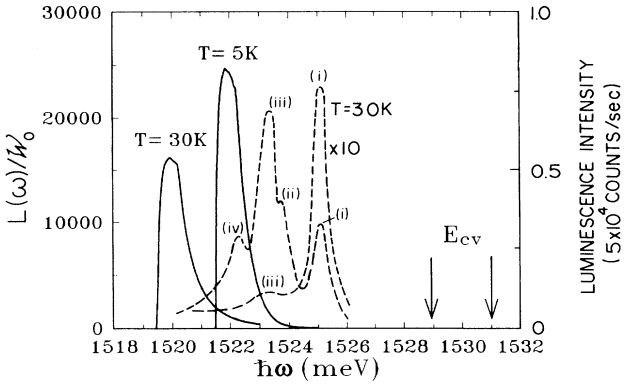

FIG. 1. Temperature dependence of the theoretical (full curves) $D^\circ-h$ photoluminescence spectra (in units of $\mathcal{W}_0$; see text) from an $L=210$ Å center-$\frac{1}{3}$-doped GaAs-$Ga_{0.7}Al_{0.3}As$ quantum well. Also shown are the experimental (dashed curves) results (in counts/sec) by Liu *et al.* (Ref. 5). E_{cv} corresponds to the onset of transitions from the $n=1$ conduction subband to the $n=1$ valence subband.

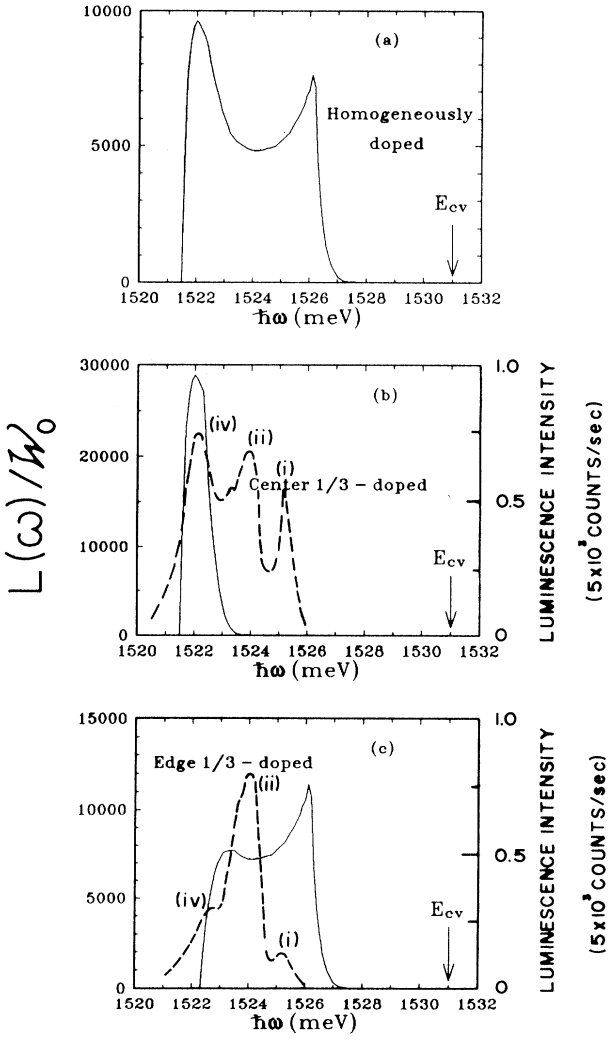

FIG. 2. $D^\circ-h$ theoretical (full curves) photoluminescence line shapes (in units of $\mathcal{W}_0$; see text) at $T=1.8$ K from an $L=210$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ quantum well with different impurity doping profiles. Also shown are the experimental (dashed curves) results (in counts/sec) by Liu *et al.* (Ref. 5). E_{cv} corresponds to the onset of transitions from the $n=1$ conduction subband to the $n=1$ valence subband.

corresponds to a "binding energy" of 10 meV] whereas the $T=30$ K theoretical $D^\circ-h$ peak is not observed in the experimental work. We have no explanation for that. We should also stress that our calculation is concerned only with the $D^\circ-h$ features of the photoluminescence spectra and, therefore, does not account for exciton, confined neutral donor-bound exciton, and confined ionized donor-bound exciton features which show up in the experimental data by Liu *et al.*[5]

The $T=1.8$ K $D^\circ-h$ theoretical photoluminescence spectra for $L=210$ Å QW's with different impurity profiles are displayed in Fig. 2 and compared with the data by Liu *et al.*[5] The "on-center" peak at $\hbar\omega=1522$ meV for the center-$\frac{1}{3}$-doped QW is in very good agreement with feature (iv) of their result for sample 3 [Fig. 3(a) of Liu *et al.*[5]], whereas for edge-doped samples the theory predicts a shift in feature (iv) to $\simeq 1523$ meV as compared to the quite minute shift in the experimental results. The theoretical peak at 1526.1 meV for edge-$\frac{1}{3}$-doped QW's [see Fig. 2(c)] is associated to the onset of transitions from on-edge donors to the valence subband and was observed as a weak feature at 1527.0 meV in sample 4 of Liu *et al.*[5]

Finally, in Fig. 3 we show the $T=1.8$ K theoretical $D^\circ-h$ photoluminescence line shapes in the case of homogeneously doped GaAs-$Ga_{0.7}Al_{0.3}As$ QW's of widths $L=80$, 140, and 210 Å. The photoluminescence spectra show essentially three features: an edge at low energies corresponding to the onset of transitions from on-center donors to the $n=1$ valence subband, a peak which we may loosely associate to "on-center" donors, and a van Hove–like peaked structure (with discontinuity of the derivative) associated to transitions involving on-edge donors. The corresponding "binding energies" associated to these features may be obtained by considering the energy shift with respect to E_{cv} (onset of conduction-to-valence transitions) and are shown in Fig. 4. Note that the full line of Fig. 4 should be compared to the experimental values (circles) in Fig. 2(a) of Ref. 5. We may add that the $D^\circ-h$ photoluminescence spectra were also calculated for the case of center-$\frac{1}{3}$-doped QW's and results for the "on-center" donor peaks were at essentially the same energy as in the homogeneously doped QW's.

Summing up, in this work we have presented a theoretical and systematic study of the $D^\circ-h$ photoluminescence spectrum from GaAs-(Ga,Al)As QW's. Typical theoretical photoluminescence line shapes show peaked structures associated to on-center and on-edge donors in good agreement with experimental results. Of course, a complete explanation of the experimental photolumines-

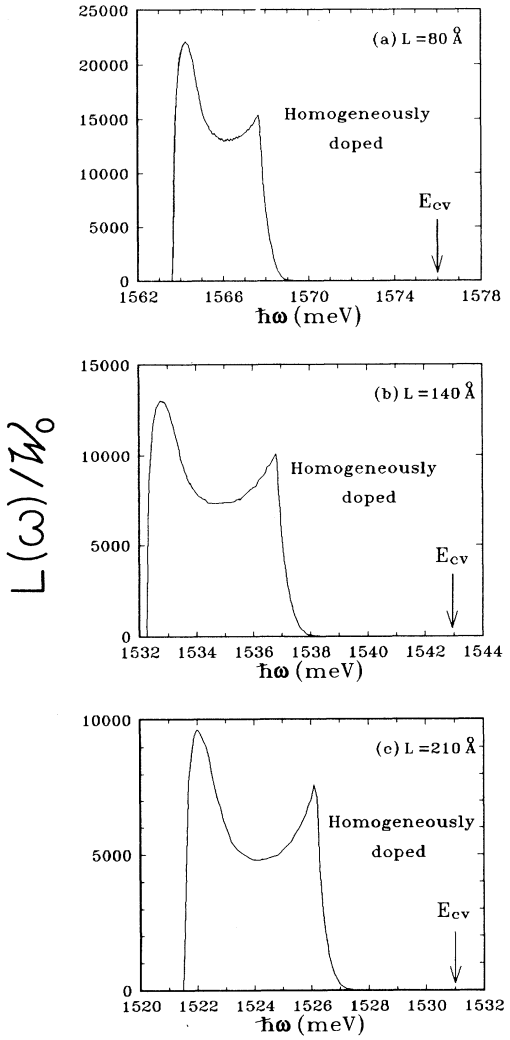

FIG. 3. $D^\circ-h$ photoluminescence line shapes (in units of $\mathcal{W}_0$; see text) at $T=1.8$ K and different well thicknesses from a homogeneously doped GaAs-$Ga_{0.7}Al_{0.3}As$ quantum well. E_{cv} corresponds to the onset of transitions from the $n=1$ conduction subband to the $n=1$ valence subband.

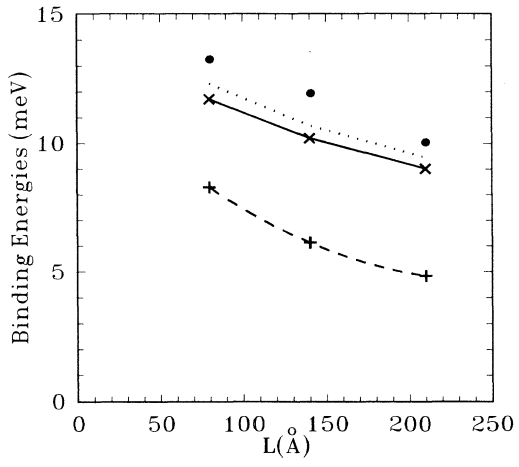

FIG. 4. Binding energies vs quantum-well thicknesses. The dotted curve corresponds to the onset of transitions from on-center donors to the valence subband, whereas the full (dashed) curve corresponds to the peak associated to on-center (on-edge) donors of the theoretical low-T $D^\circ-h$ photoluminescence spectra from GaAs-$Ga_{0.7}Al_{0.3}As$ quantum wells. Circles: experimental values corresponding to feature (iv) of the spectra by Liu *et al.* (Ref. 5).

cence line shapes as measured by Liu *et al.*[5] would involve a calculation of matrix elements of excitonic wave functions as well as neutral and ionized donor-bound exciton wave functions[15] with holes in the valence subband, which is much beyond the scope of this work.

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