Photoluminescence study of shallow acceptors in GaAs-$Ga_{1-x}Al_xAs$ cylindrical quantum-well wires

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A systematic study of the theoretical acceptor-related photoluminescence spectra in a cylindrical GaAs-(Ga,Al)As quantum-well wire is performed. The acceptor states are described within a variational scheme in the effective-mass approximation. Photoluminescence spectra associated with acceptors are calculated for both homogeneous and on-center spike-doped distributions of acceptors in the quantum-well wire. Results are dependent on the temperature, on the choice of the quasi-Fermi-energy level of the conduction-subband electron gas, and on the distribution of acceptors in the wire. The photoluminescence spectra corresponding to the on-center spike-doped Gaussian distribution (width of the doping spike of the order of 50 Å) shows a peak for energies associated with on-center impurity states, as is expected, whereas for a homogeneous distribution of acceptors in the well we essentially found an edge in the spectra associated with transitions involving on-center acceptors and a peaked structure related to the onset of transitions from the conduction subband to on-edge acceptors. Although no experimental results for GaAs-(Ga,Al)As quantum-well wires are available, our results agree qualitatively with previous theoretical and experimental work on GaAs-(Ga,Al)As quantum-well heterostructures.

I. INTRODUCTION

Low-dimensional structures[1–10] having quantum confinement in one, two, or three dimensions, such as quantum wells (QW's), quantum-well wires (QWW's), and quantum dots (QD's), have attracted both theoretical and experimental attention due to their electronic properties and to the wide-ranging potential applications in electronic devices.

The presence of impurities in these structures (intentionally doped or otherwise) contributes to additional responses when external probes are applied to these systems. In QW's, there have been experimental photoluminescence data in which, besides the excitonic peak, there is another structure in the spectra associated with the electronic transitions between the conduction-electron gas and the acceptor impurity states.[11,12] A theoretical study by Oliveira and López-Gondar[13] has suggested the existence of two features in the GaAs-$Ga_{1-x}Al_xAs$ QW's acceptor-related photoluminescence spectra, which are associated with on-center and on-edge impurity positions and which have intensities depending on experimental conditions and properties of the system, such as the temperature, the distribution of impurities in the well, and the laser intensity.

Although there have been considerable improvements in experimental techniques for the construction of QWW's, such as molecular-beam epitaxy (MBE),[6] metal-organic chemical-vapor deposition (MOCVD),[7,9] and electron-beam (EB) lithography combined with reverse mesa wet etching,[10] to date there are no experimental reports on the photoluminescence spectra associated with acceptor impurity states in QWW's. Nevertheless, due to the importance of impurities in potential device applications of heterostructures, the understanding of the properties of impurity states associated with such systems is certainly a subject of considerable technological and scientific importance.

This work reports a systematic analysis of the photoluminescence spectra associated with shallow hydrogenic acceptors in cylindrical GaAs-(Ga,Al)As QWW's. In Sec. II some of the theoretical aspects concerning the photoluminescence spectra are discussed; results and discussions are presented in Sec. III, and conclusions in Sec. IV.

II. THEORY

The transition probability per unit time for transitions from the conduction subband to a state associated with an acceptor impurity located at $\boldsymbol{\rho}_i$ in a cylindrical QWW is proportional to the square of the matrix element of the electron-photon interaction H_{int} between the wave functions of the initial state (conduction-subband electron gas) and final (impurity) states; i.e.,

$$W=\frac{2\pi}{\hbar}\sum_i |\langle f|H_{\text{int}}|i\rangle|^2\delta(E_f-E_i-\hbar\omega)\ , \tag{1}$$

with $H_{\text{int}}=C\mathbf{e}\cdot\mathbf{p}$, where $\mathbf{e}$ 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 that describes effects of the photon vector potential.[14] Following the effective-mass approximation, the above matrix element may be written as[15]

$$\langle f|H_{\rm int}|i\rangle \cong C\mathbf{e}\cdot\mathbf{P}_{fi}S_{fi} \;, \tag{2}$$

with

$$\mathbf{P}_{fi}=\frac{1}{\Omega}\int_{\Omega}d\mathbf{r}\,u_f^*(\mathbf{r})\mathbf{p}\,u_i(\mathbf{r}) \tag{3}$$

and

$$S_{fi}=\int d\mathbf{r}\,F_f^*(\mathbf{r})F_i(\mathbf{r}) \;, \tag{4}$$

where Ω is the volume of the unit cell, F_i (F_f) is the envelope function, and u_i (u_f) is the periodic part of the Bloch state for the initial (final) state. For the case of the acceptor impurity, $S_{fi}=S_{fi}(\rho_i,\lambda,k)$ is given by[16,17]

$$S_{fi}=2N_1N_2\left[\int_0^d d\rho\,\rho J_0(r_{10}^c\rho)J_0(r_{10}^v\rho)\int_0^\infty dz\cos(kz)\int_0^{2\pi}d\phi\,\Gamma(\boldsymbol{\rho},\boldsymbol{\rho}_i,z,\lambda)\right.$$
$$\left.+Q\int_d^\infty d\rho\,\rho K_0(b_{10}^c\rho)K_0(b_{10}^v\rho)\int_0^\infty dz\cos(kz)\int_0^{2\pi}d\phi\,\Gamma(\boldsymbol{\rho},\boldsymbol{\rho}_i,z,\lambda)\right] , \tag{5}$$

where

$$Q=\frac{J_0(r_{10}^c d)}{K_0(b_{10}^c d)}\frac{J_0(r_{10}^v d)}{K_0(b_{10}^v d)} \;, \tag{6}$$

$$r_{10}^{c,v}=\left[\frac{2mE_{10k}^{c,v}}{\hbar^2}-k^2\right]^{1/2} ,$$
$$b_{10}^{c,v}=\left[\frac{2m(V_b-E_{10k}^{c,v})}{\hbar^2}+k^2\right]^{1/2} . \tag{7}$$

In the above equations, J_0 and K_0 are, respectively, modified Bessel functions of the first and second kind of zero order and N_1 (N_2) is a normalization constant for the initial (final) -state wave function. $E_{10}^{c,v}$ is the ground state of the system without impurities, and the upper indices (c,v) refer to conduction and valence subbands, respectively. The effective mass m is given by $m_{c,v}$ (for the conduction or valence band), $V_b=V_b^{c,v}$ is the corresponding constant potential in the barrier material, and

$$\Gamma(\boldsymbol{\rho},\boldsymbol{\rho}_i,z,\lambda)=\exp\{-\lambda[(\boldsymbol{\rho}-\boldsymbol{\rho}_i)^2+z^2]^{1/2}\} \;, \tag{8}$$

where λ is a variational parameter, $\boldsymbol{\rho}$ is the position vector in a plane perpendicular to the cylindrical wire, and $\boldsymbol{\rho}_i$ is the acceptor position in the plane.

For a GaAs-$Ga_{0.7}Al_{0.3}As$ QWW of radius d and length L, the transition probability per unit time for conduction-to-acceptor transitions associated with a single impurity located at $\boldsymbol{\rho}_i$ is therefore given by

$$W_d(\rho_i,\omega)=W_0\left[\frac{(m_c)^{1/2}\hbar L}{2^{1/2}m_0a_0^2}\right]\times\frac{S_{fi}^2[\rho_i,\lambda,(2m_c\Delta/\hbar^2)^{1/2}]}{\Delta^{1/2}}\Upsilon(\Delta) \;, \tag{9}$$

where a_0 is the Bohr radius, m_0 is the free-electron mass, and $\Upsilon(\Delta)$ is the step function. In this expression we have

$$\Delta=\hbar\omega-\varepsilon_g+E_b(\rho_i,d) \;, \tag{10}$$

$$W_0=\frac{4m_0}{\hbar^3}a_0^2|C|^2|\mathbf{e}\cdot\mathbf{P}_{fi}|^2 \;, \tag{11}$$

where $\hbar\omega$ is the photon energy, E_b is the binding energy of the acceptor impurity, and $\varepsilon_g=E_g+E_{10}^c+E_{10}^v$, with E_g being the bulk GaAs band gap (see Fig. 1).

We consider a single GaAs-(Ga,Al)As QWW with a $P_a(\rho_i)$ distribution of acceptor impurities in which electrons have been optically injected into the conduction band and recombine with holes in the acceptor band. We also assume that the temperature is low enough to guarantee that each acceptor state is filled with a hole. The acceptor-related photoluminescence spectrum can be written as

$$L_d(\omega)=2\pi\int_0^d d\rho_i\rho_i W_d(\rho_i,\omega)P_a(\rho_i)f(E_k) \;, \tag{12}$$

where $f(E_k)=1/\{1+\exp[\beta(\Delta-E_F)]\}$ is the Fermi dis-

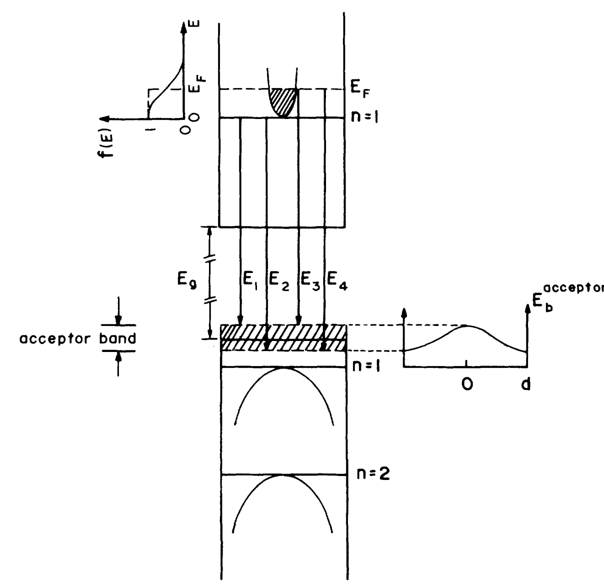

FIG. 1. Schematic representation of special luminescence transitions in a GaAs-(Ga,Al)As cylindrical QWW with an acceptor impurity band. The parabolas represent a pictorial view of the k_z dispersion of the $n=1$ conduction subband and $n=1$ and 2 valence subbands. Also shown are the Fermi distribution for the conduction-subband electron gas (on the left) and the dependence of the acceptor binding energy as a function of the impurity position (on the right).

tribution function for the conduction subband electron gas, with $\beta = 1/k_B T$ and E_F the quasi-Fermi-energy level of the electron gas, measured from the bottom of the subband.

The main results of this calculation are presented in the next section. For the case of a finite confining potential, the height of the barrier V_b is taken to be 60% (40%) of the band-gap discontinuity $\Delta E_g = 1.247x$ eV in the GaAs-$Ga_{1-x}Al_xAs$ QWW for the conduction (valence) band.[18,19] In calculating acceptor states, we used an average spherical[20] effective mass $m_c \simeq 0.30 m_0$, although a more realistic description should certainly consider the effects of the coupling of the top four valence bands.[21] All results are presented for the case of an Al concentration of $x = 0.3$, and, unless otherwise stated, the results presented are calculated using a homogeneous distribution of acceptors along the well wire $[P_a(\rho_i) = 1/\pi d^2]$.

III. RESULTS AND DISCUSSION

A schematic representation of a cylindrical GaAs-(Ga,Al)As QWW doped with a homogeneous distribution of acceptor impurities, and special photoluminescence transitions (E_1, E_2, E_3, and E_4), are shown in Fig. 1. The lower edge for photoluminescence transitions from the $n = 1$ conduction subband to the acceptor impurity band is represented by E_1, whereas E_2 corresponds to the onset of transitions associated with on-edge acceptors. At $T \to 0$, E_3 and E_4 correspond to the upper edges of transitions involving on-center and on-edge acceptors, respectively. Of course, the structures in the photoluminescence spectra associated with E_3 and E_4 will be smeared out for $T \gtrsim 25$ K due to the effect of the Fermi distribution function.

The acceptor-related theoretical photoluminescence for a GaAs-$Ga_{0.7}Al_{0.3}As$ QWW with radius $d = 100$ Å is presented in Fig. 2 for $E_F = 10$ meV and $T = 2$ K. At this low temperature, the van Hove–like structures E_3 and E_4 (see Fig. 1) are evident in the photoluminescence spectrum. The structure at E_3 (E_4) is related to transitions from the quasi-Fermi-energy level[22] of the conduction-subband electron gas to states associated with on-center (on-edge) acceptor impurities. It becomes pronounced at very low temperatures, as may be seen in Fig. 1 ($T = 2$ K). This would suggest a high-resolution photoluminescence experiment to measure the quasi-Fermi-energy level of the conduction-electron gas in the quasiequilibrium steady state.[13] One should keep in mind, however, that the photoluminescence spectra associated with the shallow acceptor band would in general appear in the low-energy "tail" of the excitonic line,[11–13] which was not considered in the present work and, therefore, features associated with the van Hove–like structures may be very difficult to observe experimentally.

Figure 3 displays our theoretical results for the photo-

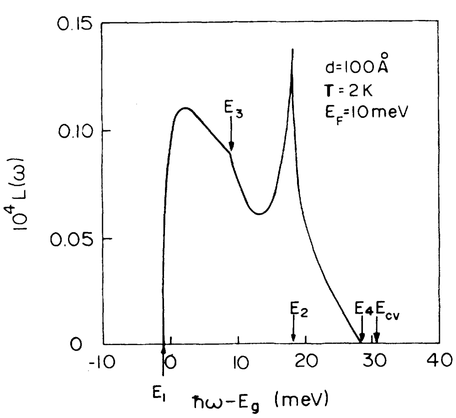

FIG. 2. Acceptor-related photoluminescence spectra (in units of W_0; see text) for a $d = 100$-Å GaAs-$Ga_{0.7}Al_{0.3}As$ cylindrical QWW in the case of $T = 2$ K and $E_F = 10$ meV. E_1 (E_2) indicates the onset of transitions from the conduction subband to the upper edge (lower edge) of the acceptor band, E_3 and E_4 indicate critical transitions associated with the quasi-Fermi-level, and E_{cv} the onset of conduction-to-valence-subband transitions.

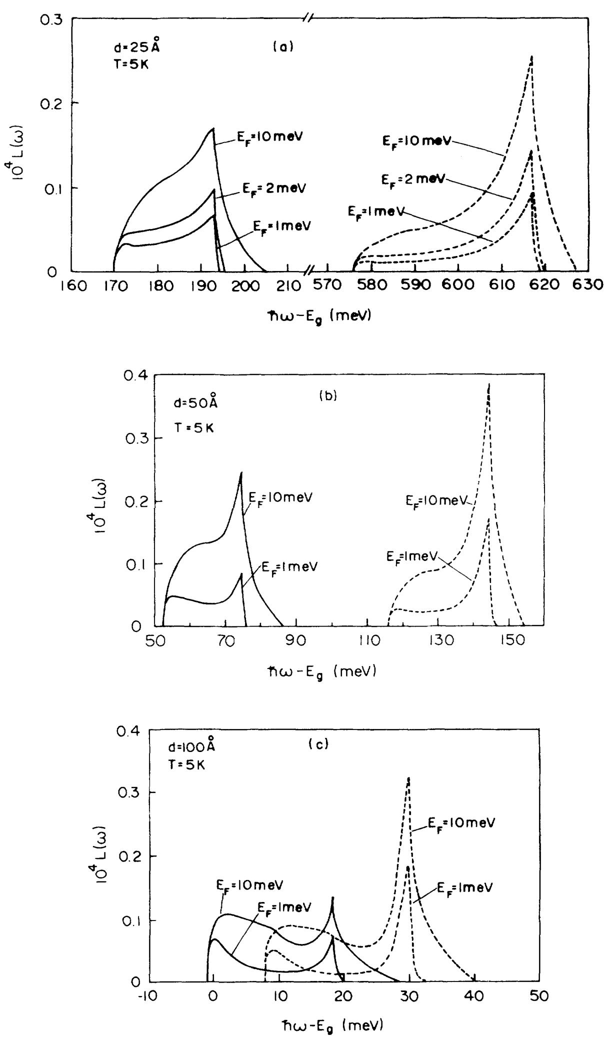

FIG. 3. Photoluminescence line shape (in units of W_0; see text) associated with electron-to-acceptor recombinations for GaAs-$Ga_{0.7}Al_{0.3}As$ cylindrical QWW's of different radii: (a) $d = 25$ Å, (b) $d = 50$ Å, and (c) $d = 100$ Å. Results are presented for both finite ($x = 0.3$; solid line) and infinite (dashed line) confinement potentials, at $T = 5$ K, and for various choices of quasi-Fermi-energy levels.

luminescence spectra for (a) $d = 25$ Å, (b) $d = 50$ Å, and (c) $d = 100$ Å GaAs-(Ga,Al)As cylindrical QWW's at $T = 5$ K and different choices of quasi-Fermi-energy levels. As was already found in the calculation of the optical-absorption spectra,[17] the finite-barrier photoluminescence curves (solid lines) show a shift to smaller energies when compared with the infinite-barrier case (dashed lines), which is easily understood by means of the changes in the $n = 1$ conduction- and valence-subband edges when a finite barrier is considered. Another feature to be pointed out is the dependence of the photoluminescence line shape on the quasi-Fermi-energy level, as may be noticed from our results. The quasi-Fermi-energy is related[22] to experimental parameters such as the laser power, the temperature, and the profile and density of the impurities, etc. We note that a common feature of all the calculated results is a peaked structure at the energy corresponding to the onset of transitions from the $n = 1$ conduction subband to the on-edge acceptor state.

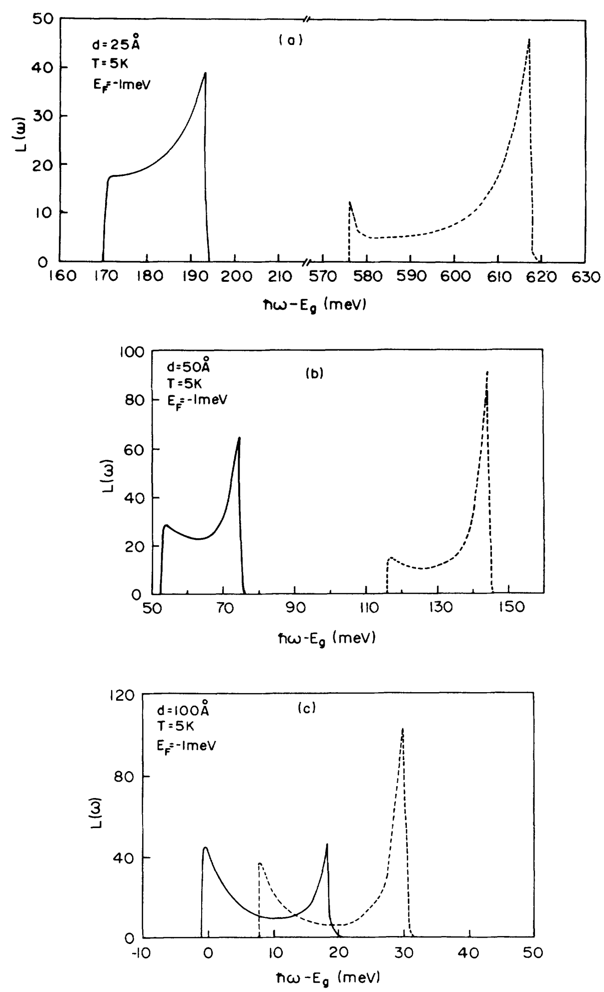

FIG. 4. Photoluminescence line shape (in units of W_0; see text) associated with electron-to-acceptor transitions for GaAs-$Ga_{0.7}Al_{0.3}As$ QWW's of different radii: (a) $d = 25$ Å, (b) $d = 50$ Å, and (c) $d = 100$ Å. Results are presented for both finite ($x = 0.3$; solid line) and infinite (dashed line) well barriers, at $T = 5$ K, and for a quasi-Fermi energy of -1 meV.

The photoluminescence line shapes for cylindrical GaAs-(Ga,Al)As QWW's of different radii, at $T = 5$ K and $E_F = -1$ meV, are shown in Fig. 4. These results are the same as one would obtain by using a Maxwell-Boltzmann distribution (instead of the Fermi-Dirac one) for the conduction electron gas, since for low temperatures and a negative quasi-Fermi-energy (or chemical potential), the electronic occupation numbers are the same in both distributions.

Besides the dependence on the quasi-Fermi-energy level and temperature, the impurity-related photoluminescence spectra depend on the acceptor distribution along the cross section of the wire as well. In order to investigate changes in the acceptor-related photoluminescence spectrum due to modifications in the impurity profile, we have also considered a spike-doped Gaussian distribution of acceptors in the wire, centered at $\rho_i = 0$, and with a 50-Å half-width. Results for both the on-center spike-doped and homogeneous distributions are presented in Fig. 5 for a cylindrical GaAs-$Ga_{0.7}Al_{0.3}As$ QWW with $d = 50$ Å, at $T = 5$ K, and for two quasi-Fermi-energies (a) $E_F = 10$ meV and (b) $E_F = 1$ meV. The photoluminescence spectra corresponding to the Gaussian distribution show a peak for energies associated with on-center impurity states as is expected, whereas the spectra corre-

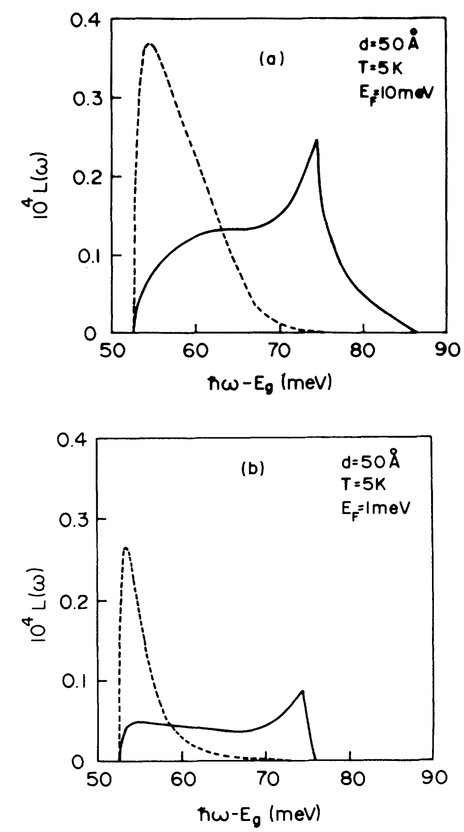

FIG. 5. Acceptor-related photoluminescence spectra (in units of W_0; see text) for a $d = 50$-Å GaAs-$Ga_{0.7}Al_{0.3}As$ cylindrical QWW, $T = 5$ K, and quasi-Fermi energies (a) $E_F = 10$ meV and (b) $E_F = 1$ meV. The solid (dashed) curves correspond to a uniform (on-center Gaussian with half-width of 50 Å) distribution of acceptor impurities.

sponding to the homogeneous distribution show a structure associated with on-edge acceptors.

IV. CONCLUSIONS

We have performed a theoretical study of the photoluminescence spectrum associated with shallow acceptors in GaAs-(Ga,Al)As QWW's. Unfortunately, to our knowledge, there are no experimental reports to date on photoluminescence spectra associated with acceptor states in QWW's. Results presented in this work may be qualitatively compared with those obtained for photoluminescence spectra associated with acceptors in GaAs-(Ga,Al)As quantum wells.[11-13] The main features of the photoluminescence line shape are quite similar in the QW and QWW cases, i.e., an edge associated with transitions involving acceptors at the center of the well, and a peak associated with transitions related to on-edge acceptors.

To sum up, in this work we have performed a systematic theoretical study of the photoluminescence spectrum associated with shallow acceptors in GaAs-(Ga,Al)As QWW's. We emphasize that the theoretical acceptor-related photoluminescence spectra depend on the distribution of impurities in the QWW and on the quasi-Fermi-energy[22] of the conduction-subband electron gas. We have calculated photoluminescence spectra for both a homogeneous and a spike-doped distribution of impurities (although we concede that these may be unrealistic in some experimental situations), and we have arbitrarily chosen quasi-Fermi-energy levels that we believe are of the proper order[22] of interest. Finally, although the present state of the art for the construction of QWW's is still in its infancy, we hope our present theoretical study will be useful in achieving a quantitative understanding of future experimental work on acceptor states in QWW's.

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