Photoluminescence line shape associated with e-A^0 acceptor-related recombination in GaAs-(Ga,Al)As quantum wells under applied electric field

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A systematic study of the e-A^0 acceptor-related photoluminescence spectra in GaAs-(Ga,Al)As quantum wells under applied electric field is presented. The approach we adopt is based on the effective-mass approximation and a variational procedure for determining the acceptor energy and envelope wave function. The impurity-related photoluminescence line shape depends on the strength of the longitudinally applied electric field, the temperature, the quasi-Fermi energy of the conduction-subband electron gas, and on the acceptor distribution along the quantum well. We find that the spectrum line shapes are essentially characterized by the presence of three features, namely, one peaked structure associated with transitions involving acceptors with binding energies at the top of the impurity band and two van Hove–like structures related to acceptors at the two edges of the quantum well.

I. INTRODUCTION

Semiconducting-heterostructure systems have been extensively investigated in the last two decades. Progress in this area has been made possible due to the development of sophisticated material-growth techniques. Today, molecular-beam epitaxy (MBE), ion-beam technology, and metal-organic chemical vapor deposition allow the realization of high-quality systems consisting of alternating layers of different materials with controlled layer thicknesses and sharp interfaces. Such man-made materials exhibit a variety of remarkable electronic properties which are due to confinement effects not present in ordinary bulk materials. As a consequence, these systems present a wide-ranging potential application in electronic devices. In particular, as GaAs and (Ga,Al)As are direct-gap, zinc-blende semiconductors with almost perfectly matched lattice parameters and band extrema at $\mathbf{k}=\mathbf{0}$, great interest has been focused on the study of (Ga,Al)As-GaAs-(Ga,Al)As quantum wells (QW's), quantum-well wires, and quantum dots.

The presence of shallow-hydrogenic impurities in low-dimensional structures gives rise to a number of phenomena which are of considerable technical and scientific relevance. Bastard[1] discussed the properties of hydrogenic states confined within a QW with an infinite potential-energy barrier. This work was followed by a series of further theoretical and experimental investigation on the subject. Recent reviews[2] present a detailed account of scientific work concerned with shallow impurities in QW's.

The physical properties of semiconducting heterostructures significantly change under externally applied electric fields as polarization of the carrier distribution and shifts of the quantum states of the system play an important role, for instance, in controlling and modulating the outputs of optoelectronic devices. Theoretically, Brum, Priester, and Allan[3] studied the binding energies of hydrogenic impurities in GaAs-(Ga,Al)As QW's under the presence of an electric field perpendicular to the interfaces (i.e., along the growth direction of the QW), Weber[4] and López-Gondar, d'Albuquerque e Castro, and Oliveira[5] calculated the electric-field-dependent density of impurity states associated with shallow donors and acceptors in infinite-, and finite-barrier QW's. In addition, in a recent work, Santiago, Oliveira, and d'Albuquerque e Castro[6] investigated the impurity-related optical-absorption spectra in GaAs-(Ga,Al)As QW's subjected to an externally applied electric field. Experimentally, Miller and Gossard[7] studied some effects of a longitudinal electric field on the intrinsic and extrinsic photoluminescence of Be-doped GaAs-(Ga,Al)As multiple-quantum-well samples grown by MBE.

The present work is concerned with the effects of applied electric fields along the growth direction of the QW on the photoluminescence line shape associated with e-A^0 acceptor-related recombination in GaAs-(Ga,Al)As QW's. In Sec. II the theory of the electric-field effects on the impurity-related photoluminescence spectra is outlined. Results and discussions are presented in Sec. III, and conclusions in Sec. IV.

II. THEORY

The Hamiltonian for a shallow acceptor in a GaAs-(Ga,Al)As QW with an applied electric field $\mathbf{F}$ parallel to

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the z-growth direction of the heterostructure may be written as

$$H=-(\hbar^2/2m_v^*)\nabla^2-\frac{e^2}{\varepsilon[\rho^2+(z-z_1)^2]^{1/2}}+V_b\theta(z^2-L^2/4)+|e|Fz\ . \tag{2.1}$$

The z origin is taken at the center of the well and the energy origin at the bottom of the GaAs conduction band. The impurity position along the growth axis is denoted by z_i, and $r=[\rho^2+(z-z_i)^2]^{1/2}$ with $\rho=(x^2+y^2)^{1/2}$ is the distance from the carrier to the acceptor site. V_b is the band offset equal to[8,9] 0.4 times the band-gap discontinuity,[10] $\Delta E_g=1.247x$ eV for the valence band; $m_v^*=0.33m_0$ (m_0 is the free-electron mass) is a spherical carrier effective mass[11] which gives a bulk value of 26 meV for the acceptor binding energy[5,12,13] and is considered constant across the interfaces; and $\theta(z)$ is the Heaviside unit-step function. We disregard the mismatch of the dielectric constant of the two materials and assume that $\varepsilon=13.1$.[14] One should note that the field F appearing in Eq. (2.1) is the *internal* screened electric field. We neglect tunneling effects due to the presence of the electric field.

The ground-state wave function and energy of the above Hamiltonian can be obtained approximately using a variational procedure. A convenient choice for the trial envelope wave function ψ is given[1] by the normalized product of the ground-state wave function $\phi_0^v(z)$ for the QW in the absence of the impurity and a hydrogenic s-wave function $\exp(-\lambda r)$, in which λ is taken as the variational parameter. The optimal value of λ is determined[5] by minimizing the expectation value $\langle\psi|H|\psi\rangle$. The acceptor binding energy is then defined as

$$E_i=E(L,z_i)=E_0-\langle\psi|H|\psi\rangle\ , \tag{2.2}$$

where E_0 is the QW ground-state energy of the $n=1$ valence subband in the presence of the applied electric field and without the impurity, which is given by the lowest root of the transcendental equation[15] (2.8) in López-Gondar, d'Albuquerque e Castro, and Oliveira.[5]

We are interested in calculating the transition probability per unit time $W_L(L,z_i)$ for conduction-to-acceptor transitions (associated to a single impurity located at $z=z_i$) which can be obtained[16] from the matrix element of the electron-photon interaction $H_{\rm int}$ between the wave functions of the initial ($n=1$ conduction subband) and final (acceptor) states, with $H_{\rm int}=C\mathbf{e}\cdot\mathbf{p}$, 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 which contains the photon vector potential. Therefore, for a GaAs-(Ga,Al)As QW of width L, we can write[17,18]

$$W_L(z_i,\omega)=W_0\frac{1}{2}\left[\frac{m_c^*}{m_0}\right]\left[\frac{1}{a_0^2}\right]S^2[z_i,\lambda,k_\perp(\omega)]\theta(\Delta)\ , \tag{2.3}$$

where a_0 is the Bohr radius, and

$$\Delta=\hbar\omega-\varepsilon_g+E(L,z_i)\ , \tag{2.4a}$$

$$k_\perp(\omega)=(2m_c^*\Delta/\hbar^2)^{1/2}\ , \tag{2.4b}$$

$$\varepsilon_g=E_g+E_{n=1}^c+E_{n=1}^v\ , \tag{2.4c}$$

$$W_0=\frac{4m_0}{\hbar^3}a_0^2|C|^2|\mathbf{e}\cdot\mathbf{P}_{fi}|^2\ . \tag{2.4d}$$

In the above equations, E_g is the bulk GaAs gap, $E_{n=1}^c$ ($E_{n=1}^v$) is the bottom (top) of the first conduction (valence) subband, $\mathbf{P}_{fi}$ is a matrix element of the momentum operator,[17] and $S[z_i,\lambda,k_\perp(\omega)]$ is given by

$$S[z_i,\lambda,k_\perp(\omega)]=\frac{2\pi N_i^v N_c}{\beta^3\lambda}\int_{-\infty}^{\infty}dz[1+\beta|z-z_i|]\times\phi_0^c(z)\phi_0^v(z)e^{-\beta|z-z_i|} \tag{2.5}$$

with

$$\beta=\beta(k_\perp)=(k_\perp^2+\lambda^{-2})^{1/2}\ , \tag{2.6}$$

and N_i^v and N_c are the normalization factors for the acceptor envelope wave function and the first conduction subband, respectively.

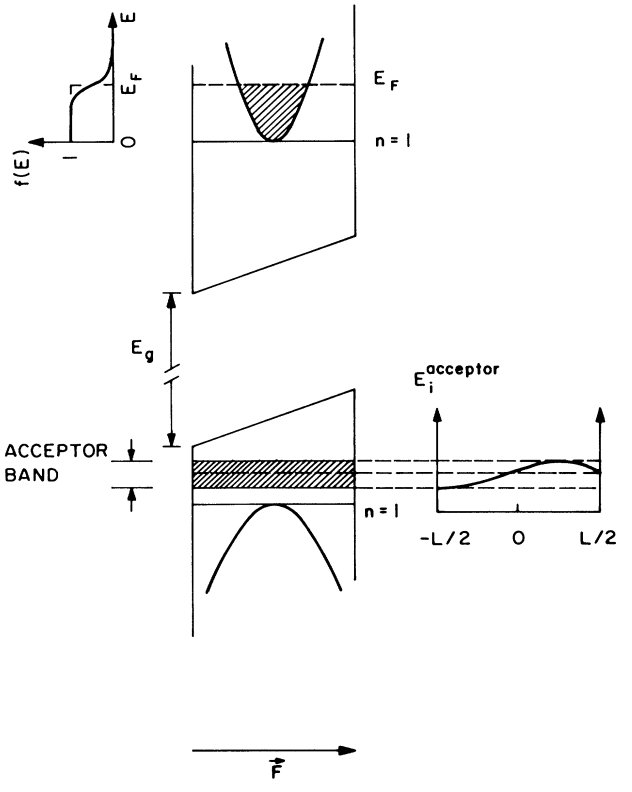

FIG. 1. Schematic representation of a GaAs-(Ga,Al)As QW with an acceptor-impurity band and submitted to a constant electric field. The parabolas represent a pictorical view of the $\mathbf{k}_\parallel$ dispersion of the $n=1$ conduction and valence subbands. Also shown are the Fermi distribution for 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).

We assume an $n_A(z_i)$ density of noninteracting acceptor impurities per unit of volume and consider a QW in which electrons have been optically injected into the conduction band and recombine with holes in the acceptor or valence bands (see Fig. 1). We are concerned with the line shape of the recombination associated with holes in the acceptor band and we assume that the temperature is low enough ($T \ll 300$ K) such that each acceptor state is filled with a hole. The photoluminescence spectrum associated with the $n=1$ conduction subband to neutral acceptor transitions (e-A^0 recombination) is therefore given by

$$L(\omega)=\frac{1}{L}\int_{-L/2}^{L/2} dz_i n_A(z_i) W_L(z_i,\omega) f(\varepsilon_k) , \qquad (2.7)$$

with $f(\varepsilon_k)=1/\{1+\exp[(\hbar\omega-\varepsilon_g+E_i-E_F)/k_BT]\}$ is the Fermi occupation number for the conduction-subband electron gas, and E_F is the quasi-Fermi-energy level[19] (measured from the bottom of the $n=1$ conduction subband) of the electron gas in the steady-state quasiequilibrium.

III. RESULTS AND DISCUSSION

Results for the e-A^0 acceptor-related photoluminescence spectra are shown in Fig. 2 for an $L=50$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW, at $T=5$ K, for a quasi-Fermi-level, $E_F=-1$ meV, and for different applied electric fields. Unless otherwise stated, calculations were performed by considering a homogeneous distribution of acceptors inside the QW, i.e., $n_A(z_i)=1$. The quasi-Fermi-level associated to the electron gas in the conduction subband may be calculated through a balance equation for the carrier density in the steady-state quasiequilibrium, with results[19] indicating that at low temperatures ($T \lesssim 10$ K) E_F is less than $\simeq 1$ meV for high laser intensities ($\simeq 10^4$ W/cm^2) and of the order of -1 meV for low laser intensities. In such regimes, the overall features of the acceptor-related photoluminescence spectra and their dependence on the applied electric field are not very sensitive to the value of E_F, only the intensity being modified due to corresponding changes in the carrier density with E_F. The spectra are essentially characterized by the presence of three features, namely, one peaked structure associated to transitions involving acceptors with binding energies E_i^{acceptor} at the top of the impurity band (cf. Fig. 1) and two van Hove–like structures (with discontinuity of the derivative) related to acceptors at the two edges of the QW. The "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. 3 as functions of the applied electric field. On the experimental ground, donor and acceptor features have been observed as extrinsic structures in photoluminescence experiments[2,12,20] in GaAs-(Ga,Al)As QW's in the absence of an applied electric field; theoretical discussions[2,18,21] of some of these results have been reported in the literature. The effects of applied electric fields on the impurity-related photoluminescence have been studied by Miller and Gossard,[7] although in their work the electric-field conditions were not well established. With recent progress in experimental techniques, we believe that the precise dependence of the acceptor-extrinsic features in the photoluminescence spectra with electric field (as presented in Fig. 3) may be obtained.

Significant changes in the e-A^0 acceptor-related photoluminescence spectra may be observed when QW's of

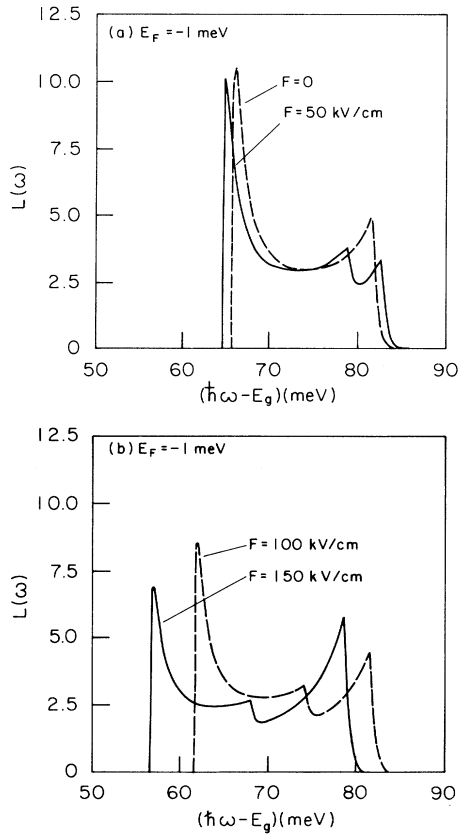

FIG. 2. Acceptor-related photoluminescence line shapes (in units of W_0—see text) for an $L=50$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW, for $T=5$ K, a quasi-Fermi-level $E_F=-1$ meV, and different electric fields.

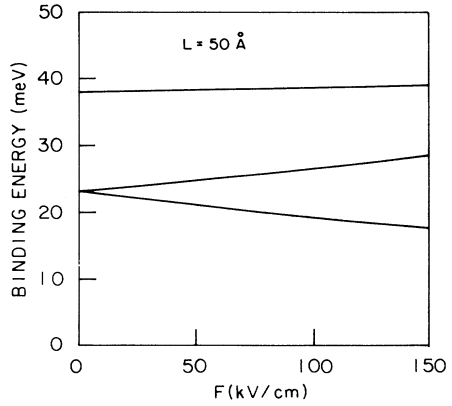

FIG. 3. Acceptor binding energies (corresponding to features in the e-A^0 photoluminescence spectra) vs the internal screened electric field F for an $L=50$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW.

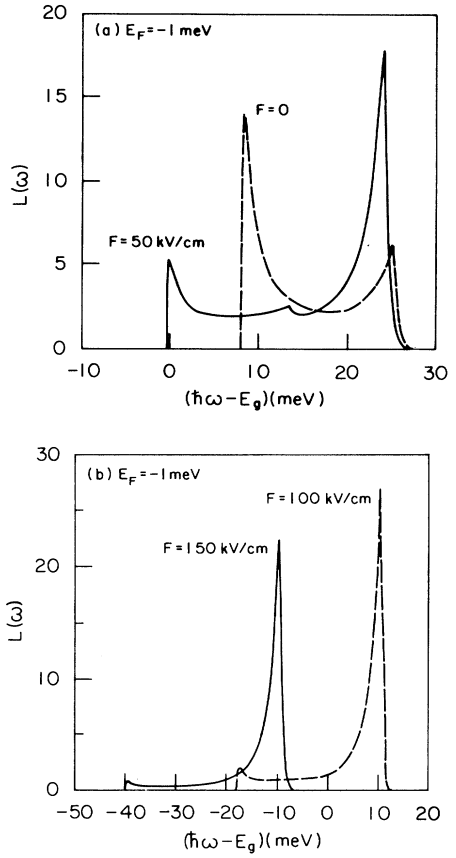

FIG. 4. Acceptor-related photoluminescence spectra (in units of W_0—see text) for an $L=100$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW, for $T=5$ K and a quasi-Fermi-level $E_F=-1$ meV; results are shown for different electric fields.

different widths are considered. Calculated results for an $L=100$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW, at $T=5$ K, for a quasi-Fermi-level $E_F=-1$ meV and for different applied electric fields are presented in Fig. 4. As the magnitude of the applied electric field increases, there is a decrease in the weight of the two structures related to transitions involving acceptors with binding energies E_i^{acceptor} at the top of the impurity band and acceptors near the right edge of the well (cf. Fig. 1). In fact, for $F=100$ and 150 kV/cm, the van Hove–like singularity associated to right-edge acceptors has essentially disappeared.

IV. CONCLUSIONS

In conclusion, we have presented in the present work a systematic study of the e-A^0 acceptor-related photoluminescence spectra in GaAs-(Ga,Al)As QW's under applied electric field. Calculations were performed within the effective-mass approximation and by using a variational procedure for determining the acceptor energy and envelope wave function. The impurity-related photoluminescence line shape depends on the strength of the longitudinally applied electric field, the temperature, the quasi-Fermi-energy of the conduction-subband electron gas, and on the acceptor distribution along the QW. We have shown that the spectrum line shapes are essentially characterized by the presence of three features (occurring at energies depending on the electric field), namely, one peaked structure associated to transitions involving acceptors with binding energies at the top of the impurity band and two van Hove–like structures related to acceptors at the two edges of the QW. We believe that the present calculation may be of importance in the quantitative understanding of future experimental work on the dependence of the acceptor-extrinsic features in the photoluminescence spectra with electric field.

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