Acceptor-Related Photoluminescence Spectra in GaAs-(Ga,Al)As Quantum Wells: Electric Field and Doping Profile Effects

Rosana B. Santiago
Centro Brasileiro de Pesquisas Físicas, Rua Xavier Sigaud 150
Rio de Janeiro, 22.290, Brazil

J. d'Albuquerque e Castro
Instituto de Física, Universidade Federal Fluminense
Niterói, Rio de Janeiro, 24.020, Brazil

Luiz E. Oliveira
Instituto de Física, Universidade Estadual de Campinas-Unicamp
C.P. 6165, Campinas, São Paulo, 13.084-110, Brazil

Received July 12, 1993

The $e - A^0$ acceptor-related photoluminescence spectra in GaAs-(Ga,Al)As quantum wells under applied longitudinal electric fields are obtained for different doping profiles within the well. Calculations are based on the effective-mass approximation and the variational method for determining the acceptor binding energy and envelope wave function. Results show that the positions and intensities of the structures in the spectrum lineshapes are sensitive to both the field strength and the acceptor distribution within the quantum well indicating that the applied electric field can be used to probe the asymmetry of the impurity distribution within the well.

Nowadays, molecular-beam epitaxy (MBE), ion-beam technology, and metal-organic chemical vapor deposition (MOCVD) 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 wide-ranging potential application in electronic devices.

The presence of shallow - hydrogenic impurities[1] in low - dimensional structures give rise to a number of phenomena which are of considerable technical and scientific relevance. Recent reviews[2] present a detailed account of scientific work concerned with shallow impurities in quantum wells (QWs). The physical properties of semiconducting heterostructures significantly change under externally applied electric fields as potential quantum states of the system play an important role, for instance, in controlling and modulating the outputs of optoelectronic devices. Theoretically, Brum et al.[3] studied the binding energies of hydrogenic impurities in GaAs-(Ga,Al)As QWs under the presence of an electric field perpendicular to the interfaces. Weber[4] and López-Gondar et al.[5] calculated the electric-field-dependent density of impurity states associated with shallow donors and acceptors in infinite- and finite-barrrier QWs. In addition, in a recent work, Santiago et al.[6] investigated the impurity-related optical absorption spectra in GaAs-(Ga,Al)As QWs 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 multiquantum well samples grown by MBE.

The present work is concerned with the effects of growth direction of the QW on the photoluminescence lineshape associated with $e - A^0$ acceptor-related recombination in GaAs-(Ga,Al)As QWs

The Hamiltonian for a shallow acceptor in a GaAs-(Ga,Al)As QW with an applied electric field **F** paralell to the z-growth direction of the heterostructure may be written as

$$\begin{aligned} H &= -(\hbar^2/2m_v^*)\nabla^2 - \frac{e^2}{\epsilon[\rho^2 + (z - z_i)^2]^{1/2}} \\ &+ V_b\theta(z^2 - L^2/4) + |e|Fz. \end{aligned} \quad (1)$$

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 an spherical carrier effective mass - we neglect the effect of coupling of the top four valence bands[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 Heavyside unit-step function. We disregard the mismatch of the dielectric constant of the two materials and assume that $\epsilon = 13.1$ (Ref. 14). One should note that the field F appearing in Eq.(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[5] 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 by minimizing the expectation value $< \psi|H|\psi >$. The acceptor binding energy is then defined as

$$E_i = E(L, z_i) = E_0 - < \psi|H|\psi >, \quad (2)$$

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 a transcendental equation (Eq.(2.8) in López-Gondar et al.[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_{int} between the wave functions of the initial (n = 1 conduction subband) and final (acceptor) states, with $H_{\text{int}} = C\mathbf{e}.\mathbf{p}$, where **e** is the polarization vector in the direction of the electric field of the radiation, **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]

$$\begin{aligned} W_L(z_i, \omega) &= W_0\frac{1}{2}\left(\frac{m_c^*}{m_0}\right)\left(\frac{1}{a_0^2}\right) \\ & S^2(z_i, \lambda, k_\perp(\omega))\theta(\Delta) \end{aligned} \quad (3)$$

where a_0 is the Bohr radius, and

$$\Delta = \hbar\omega - \epsilon_g + E(L, z_i), \quad (4.a)$$

$$k_\perp(\omega) = (2m_c^*\Delta/\hbar^2)^{1/2}, \quad (4.b)$$

$$\epsilon_g = E_g + E_{n=1}^c + E_{n=1}^v, \quad (4.c)$$

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

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 $S(z_i, \lambda, k_\perp(w))$ is given by

$$\begin{aligned} S(z_i, \lambda, k_\perp(\omega)) &= \frac{2\pi N_i^v N_c}{\beta^3\lambda} \\ & \int_{-\infty}^{\infty} dz[1 + \beta|z - z_i|]\phi_0^c(z)\phi_0^v(z)e^{-\beta|z-z_i|} \end{aligned} \quad (5)$$

with

$$\beta = \beta(k_\perp) = (k_\perp^2 + \lambda^{-2})^{1/2}, \quad (6)$$

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

We assume an $n_A(z_i)$ density of non-interacting 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 lineshape of the recombination associated with

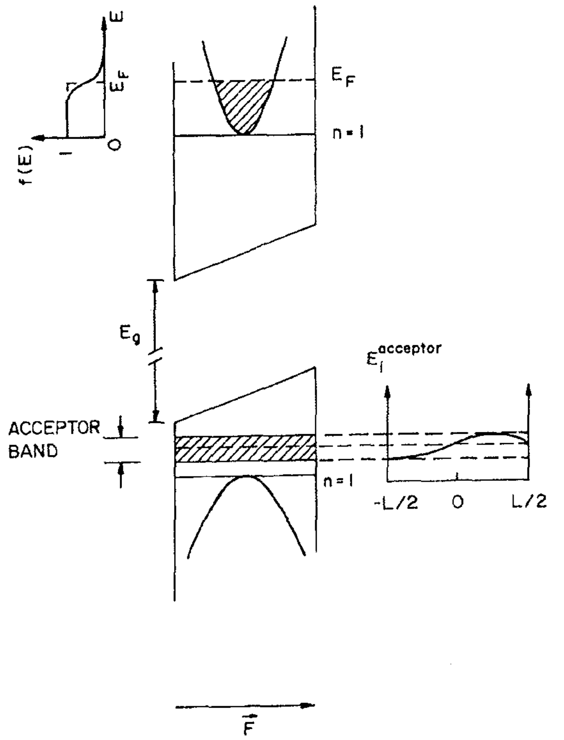

Figure 1: Schematic representation of a GaAs-(Ga, Al)As QW with an acceptor impurity band and submitted to a constant electric field. The parabolas represent a pictorical view of the $k_\parallel$ dispersion of the $n = 1$ conduction and valence subbands. Also shown are the Fermi distribution for the conduction-subband electron gas (on the left) and the dependence of the acceptor binding energy as function of the impurity position (on the rigth).

holes in the acceptor band and we assume that the temperature is low enough ($T << 300$ 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

$$L(\omega) = \frac{1}{L} \int_{-L/2}^{L/2} dz_i n_A(z_i) W_L(z_i, \omega) f(\epsilon_k), \qquad (7)$$

with

$$f(\epsilon_k) = 1/\{1 + \exp[(\hbar\omega - \epsilon_g + E_i - E_F)/k_B T]\}$$

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 quasi-equilibrium.

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 quasi-Fermi levels $E_F = -1$ and 1 meV, and for different applied electric fields. Unless otherwise stated, calculations were performed by considering an 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 quasi-equilibrium, 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 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 to 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 QWs in the absence of an applied electric field; theoretical discussion[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.

As the temperature of the sample is reduced, the energy distribution of the electrons in the conduction subband becomes sharper and, as a consequence, the structures in the impurity-related photoluminescence spectrum become more pronounced. Such an effect is il-

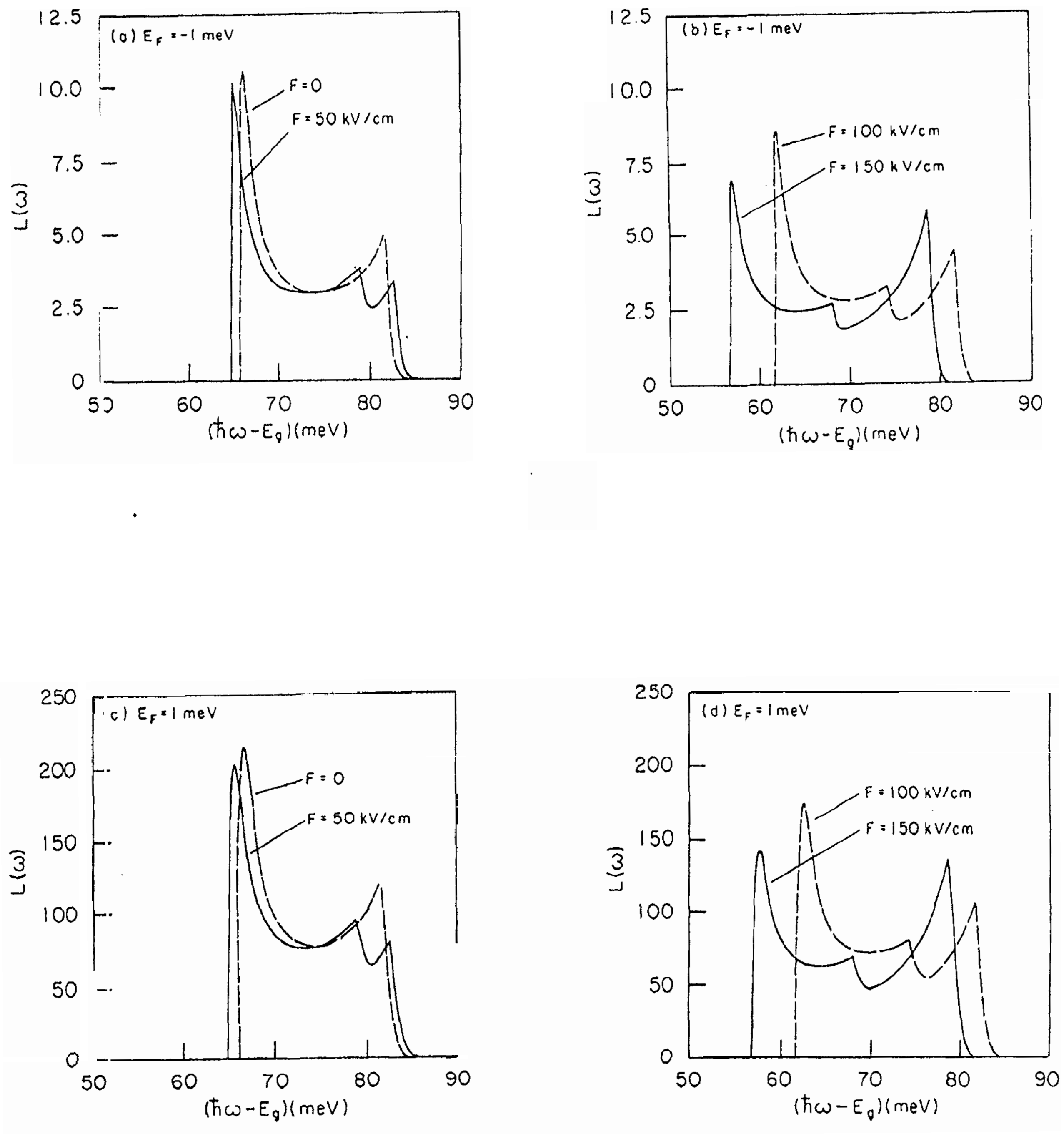

Figure 2: Acceptor-related photoluminescence line shapes (in units of W_0 - see text) for an L = 50Å GaAs-Ga$_{0.7}$Al$_{0.3}$As QW, for T = 5K, quasi-Fermi levels E_F = -1 meV [(a) and (b)] and 1 meV [(c) and (d)], and different electric fields.

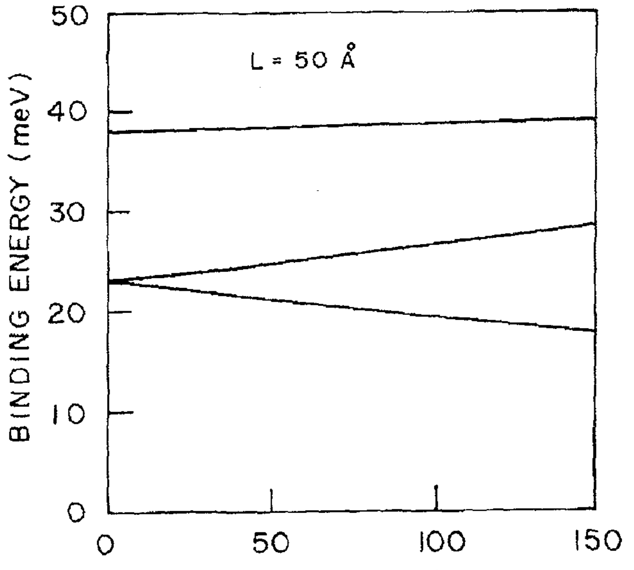

Figure 3: Acceptor binding energies (corresponding to features in the $e - A^0$ photoluminescence spectra) versus the internal screened electric field F for an L = 50 Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW.

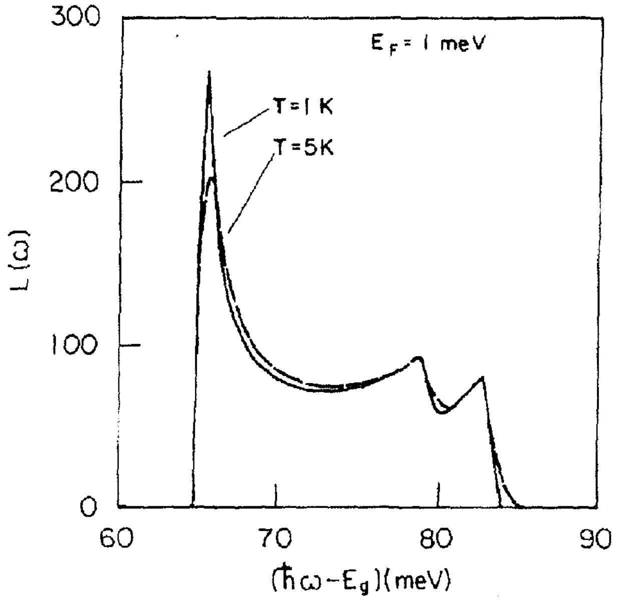

Figure 4: Photoluminescence line shapes (in units of W_0 - see text) associated with electron - to - acceptor recombinations for an L = 50 Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW, F = 50 kV/cm, E_F = 1 meV, and temperatures T = 1K (solid line) and T = 5K (dashed line).

lustrated in Fig. 4, which shows results for an L = 50Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW, with quasi-Fermi level E_F = 1 meV, internal electric field F = 50 kV/cm, and temperatures T = 1 and 5 K.

Significant changes in the e − A^0 acceptor-related photoluminescence spectra may be observed when QWs of 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 quasi-Fermi levels $E_F = -1$ and 1 meV, and for different applied electric fields are presented in Fig. 5. 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.

We present in Fig. 6 the acceptor-related photoluminescence spectra for an L = 100 Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW with impurity profiles corresponding to left and right 1/2-doped wells, for T = 5 K, quasi-Fermi level E_F = -1 meV, and electric fields F = 50 and 150 kV/cm. One may notice that the asymmetry in the impurity distribution inside the well leads to markedly different features in the photoluminescence lineshape in the presence of an externally applied electric field. In addition, as expected for the doping profiles under consideration, the average of the results for the left and right 1/2-doped wells equals the spectra previously shown in Figs. 5 (a) and 5 (b).

In conclusion, we have presented a systematic study of the $e - A^0$ acceptor-related photoluminescence spectra in GaAs-(Ga,Al)As QWs under applied electric field. The impurity-related photoluminescence lineshape 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 lineshapes in the case of a uniform impurity distribution are essentially characterized by the presence of three features (occuring 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

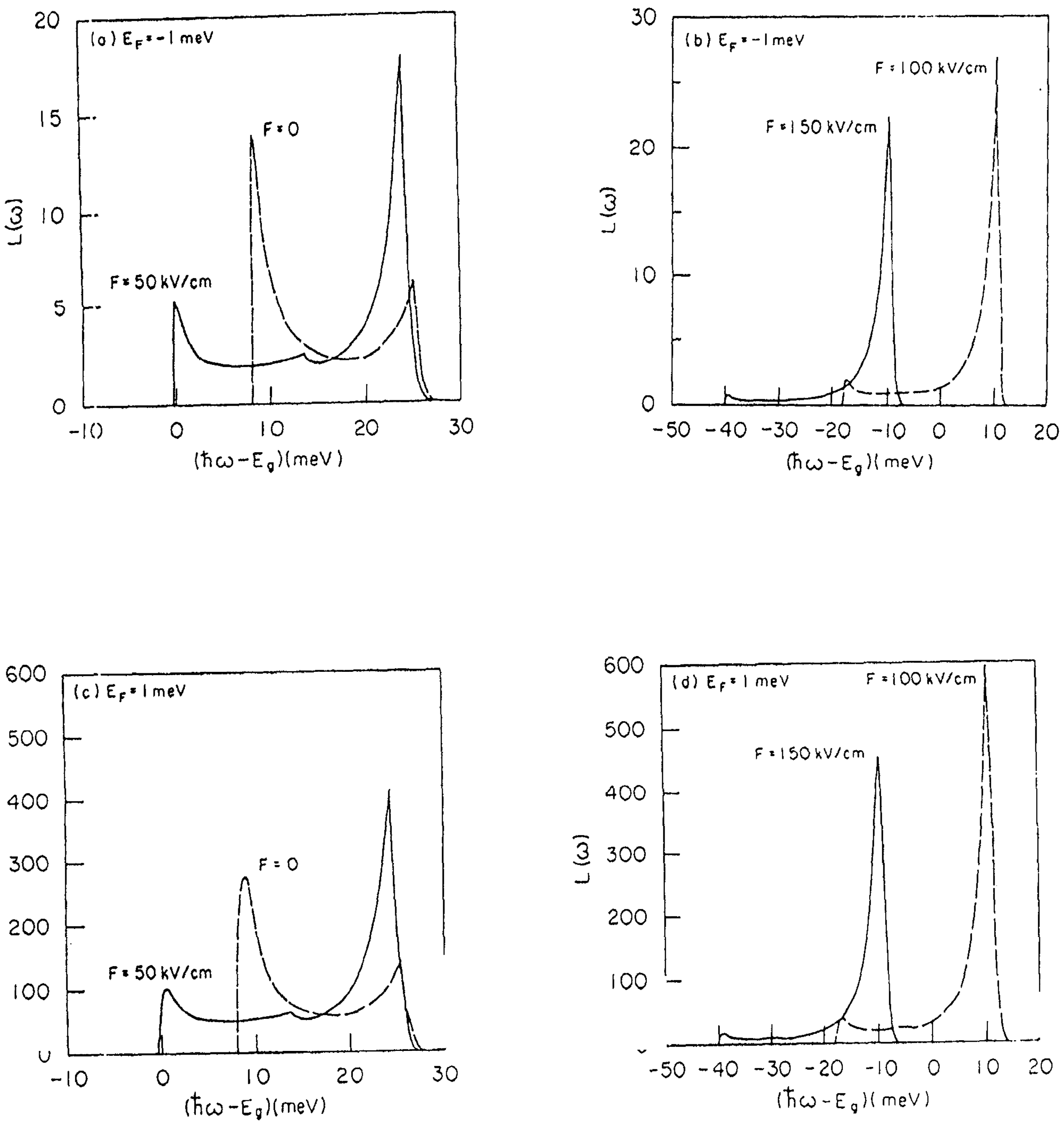

Figure 5: Acceptor-related photoluminescence spectra (in units of W_0 - see text) for an L = 100Å GaAs-Ga$_{0.7}$Al$_{0.3}$As QW for T = 5 K and quasi-Fermi levels E_F = -1 meV [(a) and (b)] and 1 meV [(c) and (d)]; results are shown for different electric fields.

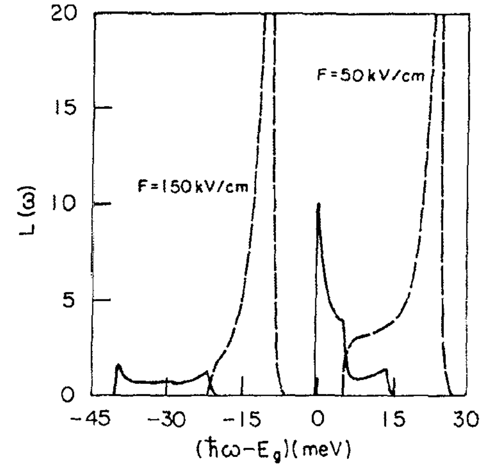

Figure 6: $e-A^0$ photoluminescence spectra (in units of W_0 - see text) at T = 5K from an L = 100Å GaAs-Ga$_{0.7}$Al$_{0.3}$As QW with $E_F = -1$ meV, and different acceptor doping profiles and applied electric fields; full (dashed) curves correspond to a left (right) 1/2 - doped QW.

two edges of the QW. Moreover, the sensitivity of the theoretical results to both the field strength and the acceptor distribution within the quantum well indicates that the applied electric field may be used to probe the asymmetry of the impurity distribution within the well.

Acknowledgments

This work was partially supported by Brazilian Agencies CNPq, FINEP, FAPESP and FAEP-UNICAMP.

References

1. G. Bastard, Phys. Rev. B**24**, 4714 (1981).
2. A. A. Reeder, J.-M. Mercy, and B. D. McCombe, IEEE J. Quant. Electr. &E-24, 1690 (1988), B. S. Yoo, L. He, B. D. McCombe and W. Schaff, Superlatt. Microstruct. **8**, 297 (1990), and references therein.
3. J. A. Brum, G. Priester and G. Allan, Phys. Rev. B32, 2378 (1985).
4. G. Weber, Phys. Rev. B**41**, 10043 (1990).
5. J. López-Gondar, J. d'Albuquerque e Castro and L. E. Oliveira, Phys. Rev. B**42**, 7069 (1990).
6. R. B. Santiago, L. E. Oliveira and J. d'Albuquerque e Castro, Phys. Rev. B 46, 4041 (1992).
7. R. C. Miller and A. C. Gossard, Appl. Phys. Lett. 43, 954 (1983).
8. R. C. Miller, D. A. Kleinmann and A. C. Gossard, Phys. Rev. B 29, 7085 (1984).
9. W. Wang, E. E. Méndez and F. Stern, Appl. Phys. Lett. 45, 639 (1984).
10. B. A. Vojak, W. D. Laidig, N. Holonyak, Jr., M. D. Camras, J. J. Coleman and P. D. Dapkus, J. Appl. Phys.**52**, 621 (1981).
11. W. T. Masselinlí, Y-C. Chang and H. Morkoc, Phys. Rev. B28, 7373 (1983).
12. R. C. Miller, A. C. Gossard, W. T. Tsang and 0 . Munteanu, Phys. Rev. B**25**, 3871 (1982).
13. A. M. White, P. J. Dean, L. L. Taylor, R. C. Clarke, D. J. Ashen and J. B. Mullin, J. Phys. C5, 1727 (1972).
14. I. Strzalkowski, S. Joshi and C. R. Crowell, Appl. Phys. Lett. 28, 350 (1976).
15. Notice a typing mistake in Eq. (2.8) of Ref. 5 which should have a plus sign in the two terms containing k_2.
16. F. Bassani and G. Pastori Parravicini, in *Electronic States and Optical* Transitions in *Solids*, edited by R. A. Ballinger (Pergamon, Oxford, 1975).
17. L. E. Oliveira and R. Pérez-Alvarez, Solid State Commun. 70, 523 (1989); Phys. Rev. B 40, 10460 (1989).
18. L. E. Oliveira and J. López-Gondar, Appl. Phys. Lett. 55, 2751 (1989); Phys. Rev. B 41, 3719 (1990).
19. G. D. Mahan and L. E. Oliveira, Phys. Rev. B **44**, 3150 (1991); L. E. Oliveira and M. de Dios - Leyva, Phys. Rev. B (in press).
20. M. H. Meynadier, J. A. Brum, C. Delalande and M. Voos, J. Appl. Phys. 58, 4307 (1985); X. Liu, A. Petrou, B. D. McCombe, J. Ralston and G. Wicks, Phys. Rev. B **38**, 8522 (1988).
21. L. E. Oliveira and G. D. Mahan, Phys. Rev. B 47, 2406 (1993).