Hole subbands in quantum wells: Comparison between theory and hot-electron-acceptor-luminescence experiments

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Recently Zachau, Kash, and Masselink [Phys. Rev. B **44**, 4048 (1991)] determined hole-subband dispersions in quantum wells experimentally with the use of hot-electron-acceptor luminescence. We present here results of multiple-band calculations, which are in very good agreement with these experiments. We also discuss the effects of subband anisotropy and its effect on the line shape. When the broadening is sufficiently small we predict a double-peak structure.

I. INTRODUCTION

Over the past decade there have been several theoretical calculations of hole-subband dispersions in two-dimensional systems such as modulation-doped interfaces, quantum wells, and superlattices. Although good agreement was found between cyclotron resonance experiments[1] and theory,[2] it was not until recently that subband dispersions were measured experimentally in a more direct way. Hayden *et al.*[3] carried out resonant magnetotunneling experiments in which the subband dispersions were mapped out. The results were in good agreement with theory, especially if the split-off band was taken into account in the calculations.[4] The same approach has also been used to investigate the anisotropy of the subband structure.[4,5]

An alternative approach was taken by Zachau, Kash, and Masselink.[6] The purpose of the present paper is a comparison with their hot-electron-acceptor-luminescence experiments, and a calculation of the line shape. In these experiments electrons were optically excited from the heavy-hole or light-hole subbands to the lowest electron subband. The transitions took place at fairly large wave vectors (of the order 5% of the distance to the Brillouin-zone boundary). Most of the hot carriers decayed by phonon emission but some of them recombined radiatively with acceptors. From the energies of the incoming and outgoing photons and a knowledge of the electron-subband structure, the hole-subband dispersions could be determined. Zachau, Kash, and Masselink studied two samples. Sample A contained 54-Å GaAs quantum wells between $Al_{0.25}Ga_{0.75}As$ barriers and for sample B the well width was 75 Å and the barriers consisted of $Al_{0.32}Ga_{0.68}As$. For both the samples the quantum wells contained acceptors and the barriers were sufficiently wide that the quantum wells could be considered as isolated. For further details the readers are referred to Ref. 6.

II. SUBBAND DISPERSIONS

The subband structure for these samples is calculated in a multiple-band envelope-function approximation. The heavy-hole, light-hole, and split-off bands are included in a 6×6 matrix, which can be decoupled into two 3×3 matrices.[7] The wave functions are matched with the use of a modified variational method, which has been described elsewhere.[8] We use the following values for the Luttinger parameters: $\gamma_1 = 6.85, \gamma_2 = 2.1, \gamma_3 = 2.9$ for GaAs,[9] $\gamma_1 = 3.45, \gamma_2 = 0.68, \gamma_3 = 1.29$ for AlAs, with a linear interpolation for the alloy. The spin-orbit splitting is $\Delta = 340$ meV for GaAs and 275 meV for AlAs. The band-gap difference between $Al_xGa_{1-x}As$ and GaAs is taken to be $\Delta E_g = 1.445x$ eV, and an offset ratio $\Delta E_v/\Delta E_g = 35\%$ is assumed. In Figs. 1(a) and 1(b) we have displayed the subband dispersions for the uppermost hole subbands for the two well widths. We have considered three cases: (a) $\phi = 0°$, where ϕ is the angle between the actual direction in the k_x-k_y plane and a $\langle 10 \rangle$ direction, (b) $\phi = 45°$ (along a $\langle 11 \rangle$ direction) and (c) the axial approximation.[2,10] In the latter case an average in the layer plane is taken but the anisotropy between the direction perpendicular to the layers and the parallel directions is taken into account. It is seen that especially the first heavy-hole subband (HH1) is quite anisotropic. In the same figures we have included the experimental results by Zachau, Kash, and Masselink.[6] As the detected photons make transitions in all directions in the Brillouin zone, one can expect the experimental results to be related to some weighted average between different directions. In the present experiments the broadening is large

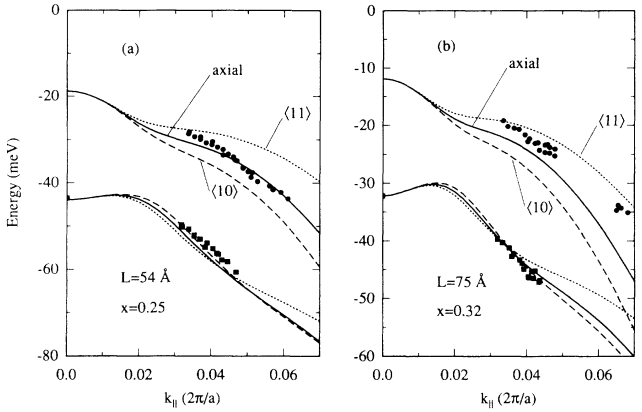

FIG. 1. Calculated and experimental subband dispersions for (a) a 54-Å, $x = 0.25$ and (b) a 75-Å, $x = 0.32$ GaAs-$Al_xGa_{1-x}As$ quantum well. The lines show the calculated dispersions for three different cases (see the text) and the dots show the experimental values. The lattice constant $a = 5.65$ Å.

enough[11] that one can expect a single peak according to the discussion in the next section. This peak should be close to the axial approximation, possibly slightly above it because of the larger density of states for $\phi = 45°$. In fact, the experimental values for HH1 are always between the calculated dispersions in the extremal directions, $\phi = 0°$ and 45°, and quite close to the results in the axial approximation. The second subband LH1 is much less anisotropic in the region of the experimental data and the calculated dispersions are in very good agreement with experiment. For this subband (especially for the 75-Å quantum well) the calculations predict an electron-like mass at small k values. Unfortunately this region is not easily accessible in the present experiments because of the much stronger luminescence of "cold" electrons. Such anomalous subbands have, however, been observed in other experiments.[3–5]

Zachau, Kash, and Masselink[6] also determined the separation between HH1 and LH1 at $k = 0$ from luminescence data. Here the agreement between theory and experiment is found to be excellent. For sample A the calculated separation is 25.1 meV and the experimental one is 24.7 meV. For sample B both theory and experiment give a separation of 20.3 meV.

We have also studied the sensitivity of the results to the input parameters. In our calculations we have considered different proposed values[9,12,13] of the Luttinger parameters which describe the bulk valence-band structure and obtained differences of a few meV. The best agreement was found for the Luttinger parameters proposed by Hess *et al.*[9] The results were found to be less sensitive to the Luttinger parameters in the barriers and the valence-band offset.

Similar calculations without inclusion of the split-off band give small but noticeable differences and slightly worse agreement with experiment. In particular, the LH-HH splitting at $k_{\|} = 0$ turns out to be overestimated when the split-off band is not included, as already noticed.[14] We have checked the calculations in this approximation using another approach[15] and obtained virtually identical results. Because the qualitative picture is independent of the inclusion of the split-off band, we have for simplicity ignored it in the discussion below of the effects of subband anisotropy.

III. EFFECT OF SUBBAND ANISOTROPY

In this section we discuss the line shape of the hot-electron-acceptor luminescence and the effect of subband anisotropy in the k_x-k_y plane ("warping"). We assume for simplicity that in the resonance region the probability of excitation does not depend on $\mathbf{k}_{\|} = (k_{\|}, \phi)$, and that the luminescence line is due to electrons which recombine before emitting phonons. For an excitation energy $\hbar\omega_L$, the line shape is determined by the probability of excitation of electrons in the first conduction subband (CB1):

$$P(\epsilon_c)\, d\epsilon_c \propto \int\int_{\epsilon_c < E_c(k_{\|},\phi) < \epsilon_c + d\epsilon_c} \delta[\, E_c(k_{\|},\phi) - E_v(k_{\|},\phi) - \hbar\omega_L]\, k_{\|}\, dk_{\|}\, d\phi, \quad (1)$$

where $P(\epsilon_c)\, d\epsilon_c$ is the number of conduction electrons with energy between ϵ_c and $\epsilon_c + d\epsilon_c$. In order to allow for broadening, we replace the δ function by a Lorentzian with full width γ. Now the main point is the following: due to the presence of a fourfold symmetry axis, the subband dispersion as a function of ϕ is periodic with period 90°, with the directions ($\phi = 0°$ and 45°) being extremal. Thus the dispersion as a function of ϕ has zero derivative there, and the values $\phi = 0°, 45°$ have more weight in the joint density of states. So, to a rough approximation, conduction electrons are mainly excited at energies corresponding to the extremal directions ⟨10⟩ and ⟨11⟩. This effect is expected to be largest for the HH1 subband, which has the greatest anisotropy in the accessible range of wave vectors.

In principle, the resulting energy difference depends on warping in both valence and conduction subbands. However, since the CB1 subband is much more dispersive than the HH1 subband, for a given excitation energy the transitions at $\phi = 0°, 45°$ involve holes with essentially the same wave vector. Thus *the energy difference of conduction electrons excited at the extremal directions is nearly equal to the HH1 warping.* This argument is confirmed by the quantitative calculation. It should be noted that the joint density of states is mainly determined by the electron-subband dispersion and therefore the larger density of states for HH1 along ⟨11⟩ compared to ⟨10⟩ only has a small effect on the peak shape.

We have evaluated expression (1) using the valence subband calculation without the split-off band, and with the same parameters as in Fig. 1. The nonparabolicity and anisotropy of the bulk conduction band is parametrized using the expression of Rössler,[16] as described in Ref. 17: results are similar to those of Ref. 18. In Fig. 2 we show the calculated peak shape (in terms of the energy of the outgoing photons) for sample A ($L_z = 54$ Å, $x = 0.25$) for an excitation energy $\hbar\omega_L = 1.84$ eV; this is somewhat smaller than the highest

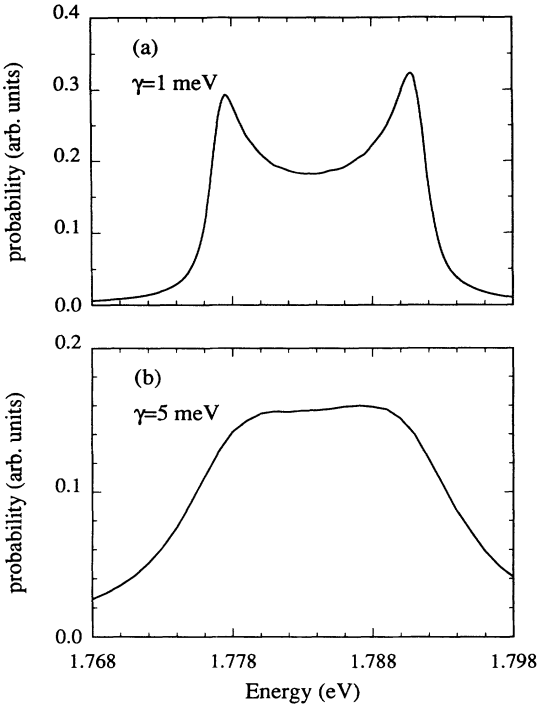

FIG. 2. Calculated peak shape in a 54-Å GaAs-$Al_{0.25}Ga_{0.75}As$ quantum well, for an excitation energy $\hbar\omega_L$ = 1.84 eV and for two different values of the broadening.

value for the HH1 recombination line. The difference between the HH1 energies in the extremal directions is $\sim$ 15 meV at the wave vectors involved [$k_{\|} \sim 0.06\,(2\pi/a)$]. A double-peak structure is evident for a broadening $\gamma = 1$ meV. For $\gamma = 5$ meV the two peaks merge into one, which has a squarelike shape and whose width is much larger than the broadening introduced. The broadening estimated from the carrier lifetimes is about 5 meV,[11] so the experimental results should be closer to Fig. 2(b). In a more elaborate calculation in which a possible ϕ dependence of the probabilities for excitation, luminescence, and phonon emission are included, the peak shape could, however, be modified. The double-peak structure seems difficult, but not impossible, to resolve experimentally. Even if γ is larger than 1 meV, it should be possible to observe a broadening and a change of shape of the recombination peak from the HH1 excitation on increasing the excitation energy. The LH1 recombination line could be taken as a reference, since warping in the LH1 subband is too small to give an observable effect.

IV. CONCLUSIONS

We have presented the results of multiple-band envelope-function calculations of the hole-subband dispersion which are in very good agreement with the hot-electron-acceptor-luminescence experiment of Zachau, Kash, and Masselink.[6] The best agreement is obtained when the Luttinger parameters of Hess *et al.*[9] are used. For a quantitative comparison with experiment it is important to include the split-off band in the calculation. The effect of subband anisotropy on the line shape has been analyzed. For a small broadening, a double-peak structure of the recombination line from the HH1 subband is predicted, with the splitting being close to the energy difference between the $\langle 10 \rangle$ and $\langle 11 \rangle$ extremal directions in the HH1 dispersion. Thus we suggest that hot-electron-acceptor luminescence could be used as a probe of hole-subband anisotropy in quantum wells.

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