Effect of strain on a second-order van Hove singularity in AlxGa1-xAs/InyGa1-yAs quantum wells

Effect of strain on a second-order van Hove singularity in $Al_xGa_{1-x}As/In_yGa_{1-y}As$ quantum wells

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(Received 18 March 1996)

We have performed low-temperature photoluminescence and photoluminescence excitation (PLE) measurements on highly degenerate *p*-type GaAs and $In_yGa_{1-y}As$ quantum wells. In the PLE spectrum of the GaAs well, evidence of a second-order van Hove singularity in the joint density of states of the ground-state light-hole and electron bands is found. This singularity results from the equality of ground-state light-hole and electron effective masses near the Γ point, being a much more restrictive demand than the usual condition for a van Hove singularity, which requires only the equality of first derivatives of the subband dispersions. The second-order van Hove singularity gives rise to a power-law divergence at the singular point, whereas the corresponding usual van Hove singularity results in a steplike discontinuity in the joint density of states. The observed singularity could be described extremely well by a simple analytical model. The increased energy gap between light- and heavy-hole ground states in the compressively strained $In_yGa_{1-y}As$ well enhances the valence-band parabolicity, resulting in the disappearance of the van Hove singularity. Furthermore, it is shown that the anisotropic character of the heavy-hole ground state in GaAs is strongly suppressed in the $In_yGa_{1-y}As$ system. All experiments are in good agreement with our numerical modeling, based on an exact solution of the 4×4 Luttinger Hamiltonian. [S0163-1829(96)05840-7]

I. INTRODUCTION

It has been well known since the early 50s that analytic singularities in the frequency distribution $g(\nu)$ of crystal vibrations necessarily occur in infinite crystals due to the periodicity of the lattice.[1] These so-called van Hove singularities occur whenever the condition $\nabla_{\mathbf{q}}=0$ is met, and can be categorized by the signs of the second derivatives of the dispersion function $\nu(\mathbf{q})$ to all coordinates q, and the dimensionality of the crystal.[1] It was realized that the same applies for the joint density of states $J(E)$ in semiconductors, leading to singularities in the optical constants of both two-dimensional (2D) and 3D bulk semiconductors.[2] More recently, van Hove singularities have attracted attention in structures with artificial periodicity, such as transverse (normal) superlattices,[3–5] lateral superlattices,[6,7] and bilayered systems.[8]

Since the lowest light-hole state (LHO) in $GaAs/Al_xGa_{1-x}As$ quantum wells (QW's) has a negative effective mass for small in-plane wave numbers, almost of the same magnitude as the electron mass, the joint density of states $J(E)$ can be expected to show a singular behavior around the LH0-$E0$ transition. This singularity will be of a much stronger nature than the ordinary van Hove singularity, since this only requires the equality of the first derivatives, $\nabla_k E_c(\mathbf{k})-\nabla_k E_v(\mathbf{k})=\mathbf{0}$. The equality of effective masses fulfills the much stronger condition $\Delta_k E_c(\mathbf{k})-\Delta_k E_v(\mathbf{k})=\mathbf{0}$, with $E_c(\mathbf{k})$ and $E_v(\mathbf{k})$ the conduction- and valance-band dispersions, respectively, and Δ the Laplace operator. Although the negative LH0 mass has been well established for a long time, both from theoretical[9] and experimental[10] studies, we are not aware of any experimental identification of this second-order van Hove singularity. Only recently, Winkler[11] predicted a logarithmic van Hove singularity in the free-electron-hole absorption spectrum of $Al_xGa_{1-x}As/GaAs$ quantum wells.

In this paper we will show clear experimental evidence of this second-order van Hove singularity in the photoluminescence excitation (PLE) spectrum of a highly degenerate, *p*-type, GaAs quantum well. The high doping concentration is necessary to suppress the exciton effects that blur the singularity in empty systems.[11] The doping has to be of *p* type, instead of the more commonly used *n* type, in order not to make the corresponding LH0-$E0$ transitions forbidden due to *k*-space filling and momentum conservation. Furthermore we will show how strain, resulting from the incorporation of indium in the well, increases the band parabolicity and isotropy and suppresses the van Hove singularity.

In Sec. II our experimental results will be presented and discussed. Results of both a numerical and an analytical analysis will be shown in Sec. III. Section IV will summarize the paper.

II. EXPERIMENT

A. Sample description and experimental setup

In this study we will present results from two $Al_xGa_{1-x}As/In_yGa_{1-y}As$ quantum wells, with nominal indium concentrations of 0 and 10%. Both samples were grown by conventional molecular-beam epitaxy techniques on $\langle100\rangle$-oriented GaAs substrates, and consisted of a single quantum well, separated by a thin buffer layer from a short-period superlattice. Both wells are nominally 95 Å wide, and symmetrically doped with Be δ layers, which are separated from the well by 250-Å spacer layers. The GaAs well is confined by $Al_{0.45}Ga_{0.55}As$ barriers, and grown at 690 °C. The $In_{0.10}Ga_{0.90}As$ well is confined by $Al_{0.25}Ga_{0.75}As$ barriers and grown at 500 °C to avoid indium diffusion. The indium concentration is confirmed by x-ray-diffraction measure-

ments. Both samples are capped by a 170-Å GaAs layer. The carrier densities, as obtained by transport measurements at 1.4 K, are $(9.0\pm0.1)\times10^{+15}$ and $(6.0\pm0.1)\times10^{+15}$ m^{-2} for the GaAs and $In_yGa_{1-y}As$ samples, respectively. Transport mobilities for both samples are typically around 10 m^2/V s. The photoluminescence and photoexcitation (PL,PLE) spectra at 1.4 K were taken in a CryoVac ^{4}He bath cryostat in which magnetic fields up to 7 T can be generated by means of a superconducting split-pair magnet. Measurements at 4.2 K and higher temperatures were performed in a CryoVac flow cryostat. The samples were excited using normal incident light from a tunable Ti:sapphire laser, pumped by a 10-W argon laser. Typically, the output power of the Ti:sapphire laser was below 5 mW, with a spot size on the sample of approximately 3 mm^2. In order to make sure that the optical spectra were not influenced by carrier heating effects, care was taken that no change in the spectra occurred upon a decrease of excitation power. The luminescence signal was focused on the entrance slit of a Spex 0.75-m double monochromator, and detected using a cooled Hamamatsu photomultiplier connected to a Keithley dc electrometer. All experiments were performed in the Faraday configuration, and by using circular polarized light in excitation as well as in detection, unless stated otherwise.

B. Results

In Figs. 1(a) and 1(b), the PL and PLE spectra of both the GaAs and $In_yGa_{1-y}As$ quantum wells are depicted. The PL traces were taken using exciting light from the Ti:sapphire laser at 1598 meV. The traces denoted $\sigma^{\alpha\beta}$ and $\sigma^{\alpha\alpha}$ are polarization-sensitive measurements, using circular (σ) polarized light. The indices α and β denote left- or right-oriented polarizations, with $\alpha\neq\beta$. The first index denotes the polarization of the exciting light, the second that of the detected polarization. The polarized light is used to separate light- and heavy-hole (LH,HH) contributions to PL(E) spectra, where the cross ($\sigma^{\alpha\beta}$) polarization is LH sensitive, and the parallel ($\sigma^{\alpha\alpha}$) polarization is HH sensitive.[12] Due to the inversion symmetry of the quantum-well potential, spin-up and -down states are degenerate,[13] which implies the equivalence of $\sigma^{\alpha\beta}$ ($\sigma^{\alpha\alpha}$) and $\sigma^{\beta\alpha}$ ($\sigma^{\beta\beta}$).

We believe that the main luminescence line of both samples, marked *A* in Fig. 1 (GaAs: 1550.5±0.1 meV, $In_yGa_{1-y}As$: 1426.8±0.2 meV), results from a nearly free HH0-*E*0 transition. Both PL lines show a broadened shoulder, marked *B* (GaAs: 1546.5±0.2 meV, $In_yGa_{1-y}As$: 1423.9±0.2 meV), on the low-energy side. We will come back to the assignment of features *A* and *B* in Sec. II C. The luminescence intensity in the cross polarization is reduced by almost a factor of 2 with respect to the parallel polarization. This is a clear signature of the spin-memory effect,[14] commonly encountered in empty and *n*-type QW's. To our knowledge this effect has not been observed before in *p*-doped structures. The main luminescence lines of the GaAs and $In_yGa_{1-y}As$ samples have a full width at half maximum of 2.4 and 4.8 meV, respectively, showing the good quality of our samples.

The PLE traces in Fig. 1 show an apparent Moss-Burstein shift in the $\sigma^{\alpha\alpha}$ traces, corresponding to HH transitions, reflecting the filled HH0 valence band. Going from GaAs to

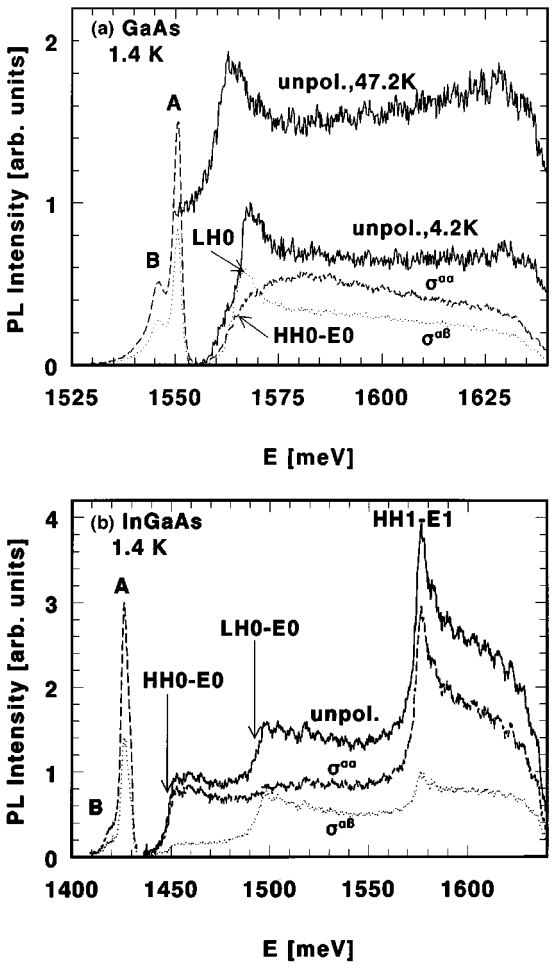

FIG. 1. Curve *A*: PL and PLE spectra of the GaAs QW. Te dashed (dotted) lines indicate parallel (crossed) polarization. The solid lines indicate unpolarized measurements. Arrows indicate PLE onsets. The feature marked LH0 is identified as a second-order van Hove singularity. Curve *B*: Same as Curve *A* for the $In_yGa_{1-y}As$ QW. The arrows indicate the PLE onsets. Note the absence of a van Hove singularity in the LH0-*E*0 transition. The peak marked HH1-*E*1 is due to excitonic enhancement. All PLE spectra are normalized on the height of the first step in the unpolarized spectrum. The 47.2-K spectrum is offset by thermal background. The intensity drop above 1630 meV is due to laser falloff.

$In_yGa_{1-y}As$ as well material, the total PLE spectrum can seen to be redshifted by some 100 meV. This is the net result of the well-known redshift due to the smaller band gap of $In_yGa_{1-y}As$, and the blueshift due to the compressive hydrostatic strain in the $In_yGa_{1-y}As$ structure. Furthermore, the energy gap between heavy- and light-hole ground states is enhanced in the $In_yGa_{1-y}As$ QW with respect to the GaAs QW, due to the shear strain. We will discuss these points in more detail in Sec. III where numerical simulations will be presented. However, the most remarkable feature in Fig. 1(a) is the peak marked LH0. We believe that this peak is the result of a second-order van Hove singularity, resulting from the negative LH0 mass around $k=0$, and that it is not a result of excitonic effects. Since our interpretation strongly differs from the common interpretation of peaklike structures near

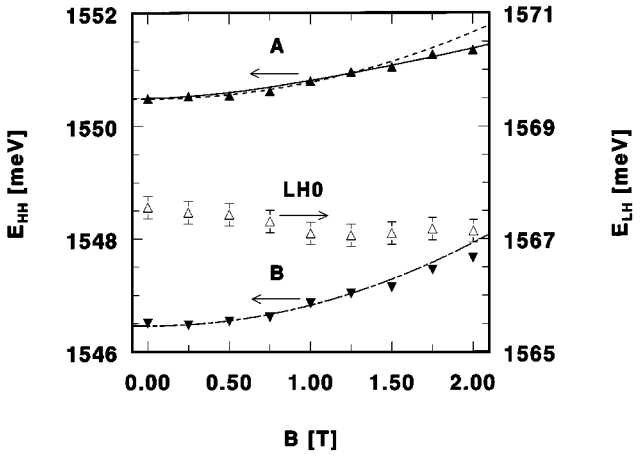

FIG. 2. Position of features A, B (left y axis), and LH0 (right y axis) vs magnetic field for the GaAs QW. The dashed and dashed-dotted lines are fits with (1) in the range 0–1 T. The solid line is the result of a more sophisticated analysis along the lines of Ref. 16, using an exciton binding energy of (0.8 ± 0.1) meV. Error bars on A and B are of the size of the markers.

the edge of an unpopulated band, we will use Sec. II C to argue why we do not attribute this peak to excitonic enhancement of transition probability. Moreover, in Sec. III we will demonstrate that this peak can be modeled without the inclusion of any Coulombic interaction between holes and electrons.

C. Excitonic effects

On qualitative grounds it can be expected that the binding energy of the HH0-$E0$ exciton ground state will be rather low in our structures, and that free band-band transitions will dominate the optical spectra. In the first place, both samples have a high 2D carrier concentration, which will screen the Coulomb interaction between the sea of (heavy) holes and the photogenerated electrons. Second, the mobilities in the wells are low compared to what is commonly found in empty or n-doped QW's. This will lead to a shorter exciton lifetime and, in consequence, to a blurred exciton spectrum. The second argument will apply for all hole subbands, whereas the first will not be generally valid due to the reduced screening efficiency of higher subbands by the ground-state heavy holes. However, the overlap between the light- and heavy-hole ground states is very strong, resulting in an efficient screening of the LH0-$E0$ exciton. These arguments can be illustrated by the PLE spectrum of the $In_yGa_{1-y}As$ QW [Fig. 1(b)]. It is obvious that both the HH0 and LH0 to $E0$ transitions do not show significant excitonic enhancement of the PLE intensity, whereas the HH1-$E1$ transition shows a clear excitonic peak at 1570 meV, which we will discuss in more detail below. Applying this reasoning to the GaAs sample leads to the conclusion that the large feature marked LH0, cannot be purely of excitonic nature.

In order to quantify our arguments about the weakness of the exciton binding energy in our samples, we performed PL(E) measurements as a function of (perpendicular) magnetic field and temperature. In Fig. 2 the energetic positions of features A, B, and LH0 of the GaAs sample are depicted as a function of magnetic field. The energies of A and B are obtained from a phenomenological lineshape analysis, using a double Gaussian fit to the PL spectrum. It is known from QW band-structure calculations for free carriers that, for low magnetic fields, the lowest HH0 Landau level is linearly dependent on magnetic field, as is the lowest $E0$ Landau level.[5] In contrast to what is thus to be expected for a purely free HH0-$E0$ transition, the main PL line (A) shows a prominent quadratic field dependence in the low-field regime. This, of course, is the expected behavior of an exciton in a weak magnetic field. In a two-dimensional system the exciton binding energy is given by[16];

$$E(B)=\left[-4+\frac{3}{8}\frac{\gamma^2}{4}\right]R_0^*, \quad \gamma=\frac{\hbar\omega_c}{2R_0^*} \tag{1}$$

where R_0^* is the effective Rydberg, and ω_c the cyclotron frequency eB/μ^*, with $\mu^*=(1/m_e^*+1/m_h^*)^{-1}$ the effective exciton mass. Fitting the energy of feature A with Eq. (1) in the range 0–1 T yields an exciton binding energy of (0.33 ± 0.04) meV, when we take $m_e^*=0.067m_0$ and $m_h^*=0.4m_0$ for the effective free electron and hole masses, respectively. As can be seen from the dashed line in Fig. 2, significant deviations arise at higher magnetic fields. Since Eq. (1) is only valid in the low-field regime ($\gamma<1$) and $\gamma\approx3$ at 1 T, the observed behavior can be more appropriately modeled with the Padé approximants of Ref. 16. These functions interpolate between the well-known analytic expressions for the exciton energy in low- and high-field regimes, and are valid for all values of γ. The result of such an analysis is also shown in Fig. 2 by the solid line. The used input parameters are the same as above. The best fit to the experimental data was obtained for an exciton binding energy of (0.8 ± 0.1) meV. This shows once more the relative unimportance of excitons at the HH0-$E0$ transition in the GaAs sample under consideration. Note that this has to be compared to similar empty QW's where binding energies around 10 meV are found. From the energetic position and field dependence, we assign the PL shoulder B to a weak acceptor-bound exciton. Assuming a Be-bound exciton, application of Haynes' rule[17] yields an estimated binding energy of 3 meV, in reasonable agreement with the observed values of 4 and 3 meV for GaAs and $In_yGa_{1-y}As$, respectively.

The field dependence of the LH0 feature in the GaAs PLE spectrum, also shown in Fig. 2, clearly reflects the nonparabolic nature of the lowest light-hole band,[15] and, as a result, does not allow us to estimate the exciton binding energy as above. However, from the lack of field dependence of the feature we can conclude that $1/m_e-1/m_{lh0}\approx0$. This implies the equality of the electron and light-hole masses, which should be the case at a singularity in their joint density of states.

Additional evidence of the irrelevance of excitonic effects to the LH0 feature can be found in temperature-dependent PLE measurements. If the LH0 peak is (partially) due to excitonic effects, a decrease in intensity is expected when the thermal energy becomes of the same magnitude as the exciton binding energy, resulting from thermal dissociation of the exciton. In Fig. 1(a) the unpolarized PLE spectra are shown at 4.2 and 47.2 K. The spectra are normalized on the

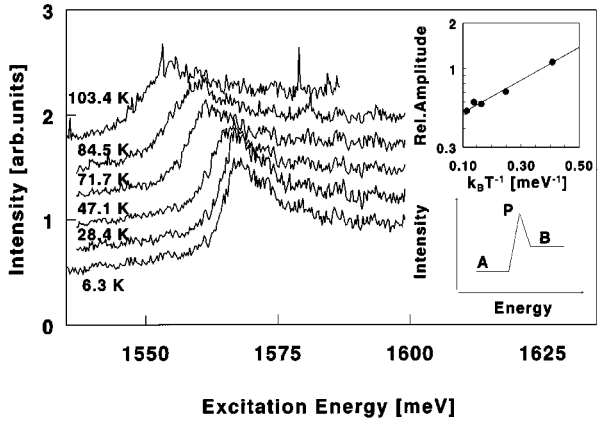

FIG. 3. Main graph: Temperature-dependent PLE spectra of the HH1-E1 transition of the $In_yGa_{1-y}As$ sample. The spectra are offset for clarity and normalized on the height of the high-energy side plateau. Upper inset: Relative amplitude of the peak in the PLE spectra vs inverse thermal energy. The solid line is a linear fit corresponding to an activation energy of 2.5 meV. Lower inset: Schematic representation of the spectra in the main graph.

height of LH0, measured from the low-energy foot of the peak to the top of the peak. The offset in the 47.2-K trace is due to the increased background of the substrate luminescence. The observed broadening of some meV is in good agreement with the thermal energy k_BT, being 4.1 meV at 47.2 K. For higher temperatures the total PLE spectrum became unobservable, due to the increasing substrate luminescence background and, probably, due to the thermal opening of nonradiative recombination channels. As can be seen from the figure, no significant change in the relative amplitude of LH0 occurs up to 50 K. This behavior can be the explained in terms of a free band-band transition, of which the van Hove singularity is a special case, or in terms of a very strong exciton, which would be the common interpretation.[18] The latter interpretation implies an exciton binding energy that exceeds the thermal energy by at least a factor 2, giving a lower bound of about 8 meV to the binding energy. The experimentally found LH0-$E0$ exciton binding energy in high-quality empty $GaAs/Al_xGa_{1-x}As$ wells of comparable width is around 11 meV.[19] It seems very unlikely to us that the binding energy in our highly degenerate sample would be almost the same as in an empty well, for reasons explained above. Therefore, we believe that the described (lack of) temperature dependence of the LH0 feature strengthens our interpretation in terms of free band-band transitions.

To enlighten the contrast between the LH0 feature and features of an excitonic nature, the HH1-$E1$ peak at 1570 meV in the $In_yGa_{1-y}As$ PLE spectrum was also studied as a function of temperature. The PLE spectra at temperatures ranging from 6.3 to 103.4 K are displayed in Fig. 3. The spectra are normalized on the height of the plateau on the high-energy side, marked B in the lower inset. Unlike the GaAs sample, the $In_yGa_{1-y}As$ sample showed no temperature-dependent background, due to the larger separation in energy between substrate- and well-luminescence lines. As is obvious from the spectra, the relative amplitude of the peaked structure, marked P in the lower inset, is strongly decreasing with increasing temperature. This is made quantitative in the upper inset of Fig. 3, in which the relative amplitude, defined as $(P-B)/(B-A)$, of the HH1-$E1$ peak is plotted logarithmically versus the inverse thermal energy. The solid line is a linear fit corresponding to an activation energy of 2.5 ± 0.1 meV. When we define the relative amplitude as $(P-A)/(B-A)$, we find a binding energy of 1.0 ± 0.1 meV. The first definition corresponds to the assumption that the excitonic peak is placed on top of the free band-band continuum, whereas the second reflects an excitonic structure that is placed in front of the continuum. Since the exciton binding energy is comparable to the spectral broadening, the correct value of the binding energy will be in between. Both results are in agreement with our interpretation of the structure in terms of excitonic enhancement of absorption intensity. The relatively low value of the obtained exciton binding energy is in good agreement with a variationally calculated value of 2.5 meV, calculated along the lines of Sugawara.[20] We used the self-consistent calculations described in Sec. III to obtain the HH1 and $E1$ wave functions and effective masses required for this calculation. No screening effects were taken into account in the calculation. The present result confirms the relative unimportance of screening by the free ground-state heavy holes of the first excited heavy-hole state. It is important to note that the LH0 feature in the GaAs spectrum at 47.2 K shows an increased relative amplitude with respect to the 4.2-K trace, independent of the exact definition of relative amplitude. Due to the temperature- and energy-dependent background, it is impossible to make this statement more quantitative.

III. SIMULATIONS

In Secs. III A and III B, we will present the results of our numerical calculations on the band structure of GaAs and $In_{0.10}Ga_{0.90}As$ quantum wells. Since our model has been described in detail in an earlier publication,[21] we will only give a brief outline of the model. In Sec. III C an analytical expression for the second-order van Hove singularity will be presented, and compared with both the numerical and the experimental results.

A. Numerical formalism

We calculated the light- and heavy-hole states, within the envelope-function approximation, as exact eigenfunctions and eigenvalues of the full 4×4 Luttinger Hamiltonian.[22] Standard flux-conserving interface conditions[23] were applied at the interfaces. The wave functions and the Coulomb potential were calculated self-consistently by iteration. The $Al_xGa_{1-x}As$ band gap is calculated using[24] $E_g(x)=1519.2+1360x+220x^2$, and the common 35:65 rule for the band-offset distribution. Strain and band offsets for the $GaAs/In_yGa_{1-y}As$ system are incorporated according to the model-solid theory of van de Walle[25] by addition of the appropriate terms on the diagonal of the Hamiltonian matrix. We used the formula of Goetz *et al.*[26] for the band gap of $In_yGa_{1-y}As$: $E_g(y)=1519.2-1583.7y+475y^2$. Electron energies and wave functions were calculated in the effective-mass approximation, using linear interpolation between the effective electron masses in GaAs $(0.067m_0)$ and InAs $(0.023m_0)$.

PLE simulations are obtained by defining a fine two-dimensional mesh in k space, with a typical grid size of 5×10^{6} m^{-1}, and two one-dimensional meshes in energy space, $\sigma^{\alpha\alpha}(E)$ and $\sigma^{\alpha\beta}(E)$, reflecting the polarized PLE spectra, with an energy step of 0.5 meV. On every k mesh-point, the optical matrix elements $M(\mathbf{k})$ of the HH_i-E_j and LH_i-E_j $(i,j=0,1)$ transitions are calculated[15] and added to the appropriate element of one of the arrays $\sigma^{\alpha\alpha}(E)$ or $\sigma^{\alpha\beta}(E)$. Here $E=E_{\mathrm{Gap}}+E_{\mathrm{hole}}(\mathbf{k})+E_{\mathrm{el}}(\mathbf{k})$, with E_{Gap} the band gap in the well, and E_{hole} and E_{el} the hole and electron energies. As a result of this definition, only momentum-conserving transitions are taken into account. The Moss-Burstein shift, reflecting the HH0 band filling, is accounted for by taking the optical matrix element equal to zero when $E_{\mathrm{HH}}(\mathbf{k})$ is smaller than the Fermi energy. The calculated spectra are slightly smoothed to reduce discretization noise. The advantage of the PLE-spectrum calculation described above over the mathematically more elegant method of Ref. 21 is its insensitivity to singularities in the joint density of states. These were found to occur for the LH0-$E0$ transition in the GaAs well. The obtained numerical resolution is beyond experimental resolution. Strictly speaking, the calculated spectrum is an absorption spectrum. However, the PLE spectrum is known to resemble the absorption spectrum closely, due to the efficient relaxation of photoexcited carriers to the Γ point, where the radiative recombination takes place.

B. Numerical results and discussion

The calculated dispersion relations of the 95 Å GaAs well, shown in Fig. 4(a), undoubtedly confirm the earlier described negative light-hole ground-state mass for small wave numbers. Quantitative analyses revealed that the LH0 and $E0$ effective masses are nominally the same for k vectors up to about $1\times10^{+8}$ m^{-1}, resulting in second-order van Hove singularity in the joint density of states, as explained in Sec. I. The extreme nonparabolicity of the LH ground state is absent in the strained $\mathrm{In}_y\mathrm{Ga}_{1-y}\mathrm{As}$ QW [Fig. 4(b)] as a result of the weaker HH-LH interaction, which, in turn, is due to the increased HH-LH separation. The $\mathrm{In}_y\mathrm{Ga}_{1-y}\mathrm{As}$ simulations are performed for an indium concentration of 11%, instead of 10%, although the latter was found in the x-ray-diffraction measurements. This was chosen in order to lessen the difference between calculated and observed transition energies. For lower indium concentrations the energetic ordering of the HH2 and LH0 bands is reversed, resulting in a sharp anticrossing near the zone center.

The PLE spectra corresponding to the dispersion curves in Fig. 4 are displayed in Fig. 5. It is obvious from a comparison with the experimental spectra in Fig. 1 that our simulations account for all features present in the ground-state transitions, including the second-order van Hove singularity at 1565 meV. This, again, confirms our claim that both HH and LH ground-state transitions can be treated as free band-to-band transitions in the heavily doped samples under consideration. In contrast, the simulated HH1-$E1$ transition in the $\mathrm{In}_y\mathrm{Ga}_{1-y}\mathrm{As}$ spectrum lacks the structure which is present in the experimental spectrum, and which must be attributed to excitonic effects.

It is worthwhile to note that not only the parabolicity of the valence bands is increased due to strain, but also the isotropy of the heavy-hole ground state, as can be deduced from the intersection of the HH0 dispersion curves in the $\langle10\rangle$ and $\langle11\rangle$ directions by the Fermi energy; see Fig. 4. This anisotropy is reflected by the steepness of the Moss-Burstein-shifted onset of HH0-$E0$ transitions in the PLE spectra (the traces marked $\sigma^{\alpha\alpha}$ in Figs. 1 and 5) by the following mechanism. In general the photon energy of a k-conserving transition is given by $E_t(\mathbf{k})=E_{\mathrm{Gap}}+E_{\mathrm{hole}}(\mathbf{k})+E_{\mathrm{el}}(\mathbf{k})$. Since the PLE onset is due to transitions at k vectors on the Fermi contour, the Moss-Burstein-shifted HH0-$E0$ onset energy becomes $E_{t,B}(\mathbf{k}_F)=E_{\mathrm{Gap}}+E_F+E_{E0}(\mathbf{k}_F)$. Because the onset in the PLE spectrum reflects an average over all k_F directions, the onset will only be sharp when $E_{t,B}$ is the same in all directions of k_F. This requires a constant magnitude of k_F in all directions, since the conduction band is isotropic. This condition can only be fulfilled for an isotropic HH0 band. In simulation as well as in experiment, the GaAs well displays a far more rounded HH0-$E0$ onset then the $\mathrm{In}_y\mathrm{Ga}_{1-y}\mathrm{As}$ well, indicating the enhanced isotropy in the strained sample.

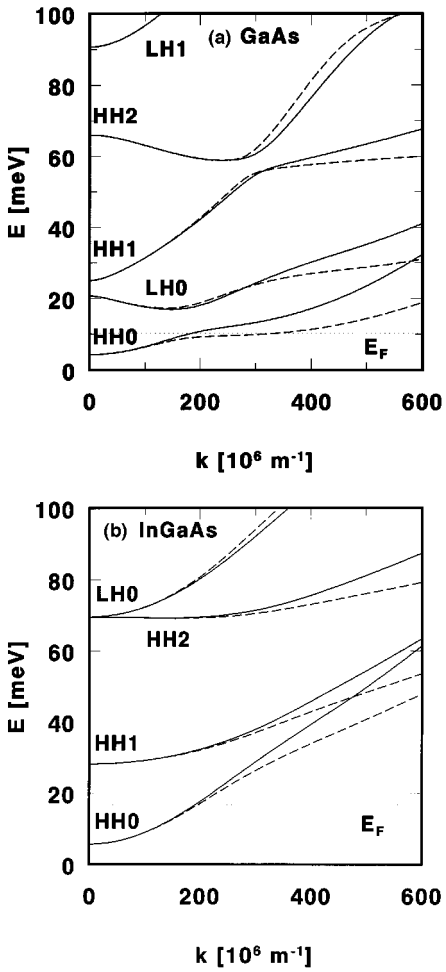

FIG. 4. Calculated dispersion relations of a 95-Å $\mathrm{Al}_{0.45}\mathrm{Ga}_{0.55}\mathrm{As/GaAs}$ QW, filled with $9.0\times10^{+15}$-m^{-2} holes (a) and a 95-Å $\mathrm{Al}_{0.25}\mathrm{Ga}_{0.55}\mathrm{As/In}_{0.11}\mathrm{Ga}_{0.89}\mathrm{As}$ QW, filled with $6.0\times10^{+15}$-m^{-2} holes (b). Solid (dashed) lines indicate the $\langle10\rangle$ ($\langle11\rangle$) direction. The $\mathrm{In}_y\mathrm{Ga}_{1-y}\mathrm{As}$ HH2 level is just below LH0 at $k=0$.

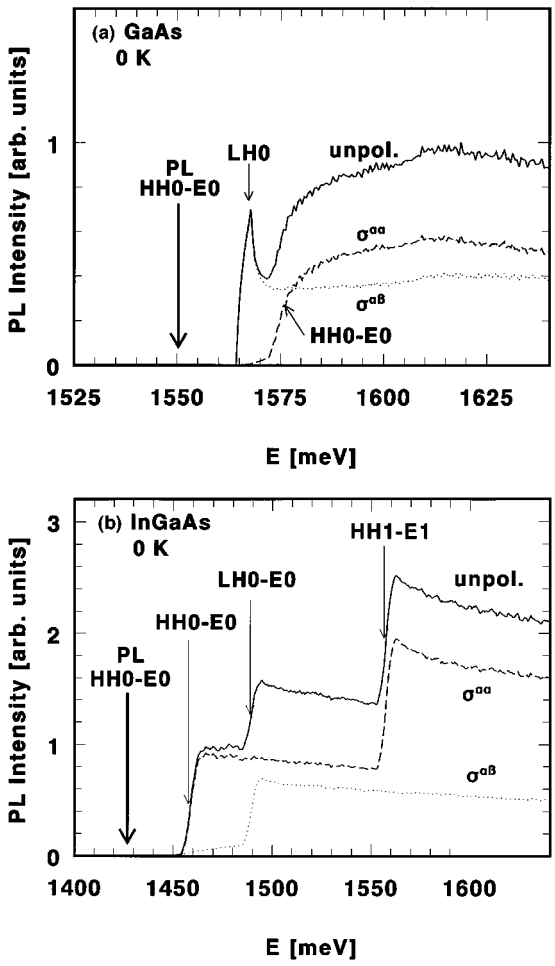

FIG. 5. Simulated PLE spectra of the GaAs (a) and $In_yGa_{1-y}As$ QW (b) of Fig. 4. Notation is the same as in Fig. 1. The fat arrows denote the position of the main PL line.

Another interesting feature in the $\sigma^{\alpha\beta}$ PLE spectrum of the $In_yGa_{1-y}As$ QW is the foot below the LH0-$E0$ onset at 1485 meV. This is a result of admixture of light-hole character in the heavy-hole ground state at nonzero wave number. This foot is also present in the experimental spectrum.

The spectra depicted in Fig. 5 are slightly redshifted in order to obtain the correct PL energy indicated by the arrows. This shift is commonly encountered in heavily doped systems, and known as band-gap renormalization, and usually described in terms of exchange- and correlation effects. The applied values for the GaAs and $In_yGa_{1-y}As$ simulations are 14.5 and 11.0 meV, respectively.

It can be noted that the predicted Moss-Burstein shift overestimates the experimentally observed shift, for both GaAs and $In_yGa_{1-y}As$ QW's. A deviation of this kind was also observed in a similar simulation of a p-doped asymmetric double quantum well.[21] In Table I we summarize the observed and predicted Moss-Burstein shifts. The Moss-Burstein shifts are calculated in two limiting situations, which will be briefly discussed in the following. The first calculation is based on full k-conservation, as are the PLE simulations in Fig. 5. This method has yielded good results for similar n-type QW's.[27] Assuming k conservation, the observed deviations in the Moss-Burstein shift have to be caused by incorrectness of the calculated dispersion relations. This is unlikely since the overall similarity of observed and calculated PLE spectra does not suggest significant errors in the calculated band structure. Moreover, the overestimation would have to result mainly from a severe incorrectness in the calculation of the very well-understood electron band, since the difference between the HH0 energies at $k=0$ and $k=k_F$ is less then the observed overestimation. The second calculation is based on full k relaxation, in which case the Moss-Burstein shift equals $E_F-E_{\mathrm{HH0}}(\mathbf{k}=\mathbf{0})$. The k-conservation selection rule could, e.g., be lifted by strong electron localization. Good results in the simulation of PL spectra of bulk semiconductors have been obtained by calculations based on this assumption.[28] Since full k relaxation strongly underestimates the Moss-Burstein shift, a partial relaxation is more likely. However, to account for the observed deviation of 10 meV, still a strong relaxation is required. As a consequence, PLE onsets and PL lines will become broadened on a similar energy scale. This is obviously not supported by the experiments. Other effects to explain the discrepancy between the calculated and observed Moss-Burstein shifts, such as nonparabolicity of the electron bands or thermal effects, are far too small to explain the deviation. Exciton effects can be ruled out since they only increase the separation between PL and PLE spectra.

TABLE I. Calculated and observed Moss-Burstein shifts. The models used for the calculations are discussed in the text. The Moss-Burnstein shifts are measured from the main PL line to the half-height of the HH0-E0 PLE onset, in the parallel polarization. The typical error is 1 meV.

Sample	Calculation		Experiment (meV)
	k-cons. (meV)	k-relax. (meV)	
GaAs	25.4	5.9	14.0
$In_yGa_{1-y}As$	32.9	10.9	21.5

It is interesting to note that a similar effect in the Moss-Burstein shift has been observed by Deppe *et al.*[29] in highly doped bulk $In_{0.53}Ga_{0.47}As$ layers. For p-type doping no appreciatable Moss-Burstein shift was found, while in n-type layers a significant shift was observed. No explanation for this effect is given by the authors. To conclude the considerations on the Moss-Burstein shift, we are unable to find a sensible explication for the overestimation, but we believe that the observed deviation is caused by a nontrivial effect. A more systematic study is, however, required to resolve this problem.

C. Analytical results

In Ref. 2 analytical expressions are derived for the various types of van Hove singularities under the usual condition of equality of the first derivatives of the electron and hole dispersions. Below we will derive an expression for an isotropic system, in which also the second derivatives of the valence and conduction band dispersion relations are equal. As we will mainly follow the lines of Ref. 2, only a brief outline of the derivation will be given.

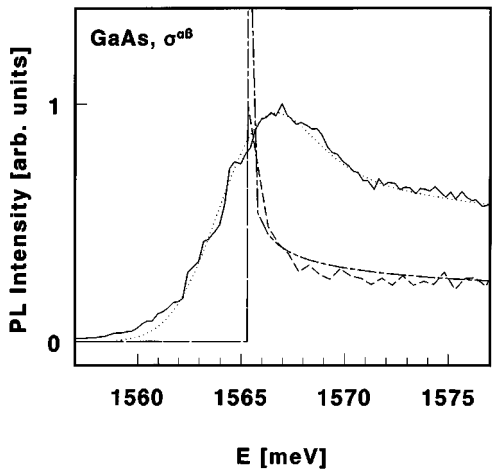

FIG. 6. Solid line: experimental PLE spectrum (normalized) of the GaAs QW in cross-polarization. Dashed line: unsmoothed numerical PLE simulation (normalized). Dash-dotted line: joint density of states $J(E)$ of LH0-E0 transition, calculated from Eq. (5) with E0=1565.3 meV, and A and B used as adjustable parameters. Dotted line: same, but convoluted with a 2.9-meV-wide Gaussian profile and normalized.

We start from the well-known expression for the joint density of states in a two-dimensional system,

$$J(E)=\frac{2}{(2\pi)^2}\int dk_x dk_y \delta(E_c(k_x,k_y)-E_v(k_x,k_y)-E), \tag{2}$$

where the integral runs over the full Brillouin zone, and E_c and E_v are conduction- and valence-band dispersion relations, respectively. Under the conditions mentioned above, we can, for an isotropic system, expand E_c-E_v around the singular point at energy E_0 as

$$E_c(k_x,k_y)-E_v(k_x,k_y)=E_0+\frac{\hbar^2}{2}\frac{k^4}{a}+O(k^6), \tag{3}$$

with $k=\sqrt{(k_x^2+k_y^2)}$. The cubic and higher odd-power contributions are zero since the dispersion relations are invariant under the transformation $k\rightarrow -k$ because of the inversion symmetry of the potential. Substitution in Eq. (2) and transformation to polar coordinates and using the property of the δ function

$$\int_a^b dx\ g(x)\delta(f(x))=\sum_{x_0} g(x_0)\left|\frac{df}{dx}\right|^{-1}_{x=x_0} \qquad (f(x_0)=0) \tag{4}$$

yields

$$J(E)=A(E-E_0)^{-1/2}+B \quad \text{if } E>E_0,$$
$$J(E)=B \quad \text{if } E<E_0, \tag{5}$$

where $A=1/(4\pi)(\hbar^2/2a)^{-1/2}$, and B a constant that depends on the detailed band structure. As is apparent from Eq. (5), a $1/\sqrt{x}$, with $x\rightarrow 0$, divergence is to be expected at the onset of the LH0-$E0$ transition in the PLE spectrum. In comparison, the usual van Hove condition gives a quadratic term in Eq. (3), and only a step in $J(E)$ at E_0.[2,30] In Fig. 6, $J(E)$, calculated from Eq. (5), is plotted, together with the numerically calculated PLE signal. Obviously there is excellent agreement between the numerical and analytical curves. Also shown are the experimental PLE signal in cross polarization and $J(E)$, convoluted with a 2.9-meV, wide Gaussian profile. Again, the similarity is striking, proving the correctness of our description.

IV. SUMMARY

In this paper we reported experimental identification of a second-order van Hove singularity in the photoluminescence excitation spectrum of a $Al_xGa_{1-x}As/GaAs$ quantum well. We showed the relative unimportance of excitonic effects in the light- and heavy-hole ground states, in both samples. We believe this is due to the efficient screening of the unpopulated LH0 state by the sea of free heavy holes. The observed spectra are in agreement with the theoretical predictions of Winkler,[11] in the sense that a singularity is found in the free-electron-hole absorption spectrum. Although Winkler identified this singularity as a logarithmic van Hove singularity, fulfilling the usual condition $\nabla_k E_c(\mathbf{k})-\nabla_k E_v(\mathbf{k})=\mathbf{0}$, we have shown that it fulfills the far more restrictive condition $\Delta_k E_c(\mathbf{k})-\Delta_k E_v(\mathbf{k})=\mathbf{0}$, which gives rise to a $1/\sqrt{x}$, with $x\rightarrow 0$, divergence. The derived analytical expressions were found to be in excellent agreement with both the numerical and the experimental results.

It is interesting to note that Gravier *et al.*[31] observed a similar structure in the cross-polarization PLE spectrum of a 80-Å p-type QW. The authors attribute this peak to excitonic effects. Although the carrier density in their sample is a factor 3 lower than in ours, we still feel that this feature can also be a van Hove singularity.

Furthermore, it was experimentally shown how the strain in an $Al_xGa_{1-x}As/In_yGa_{1-y}As$ QW increases the band parabolicity, which translates into the elimination of the second-order van Hove singularity. From the steepness of the Moss-Burstein-shifted onsets of the HH0-$E0$ transitions in PLE, it was deduced that the severe warping of the heavy-hole ground state in the GaAs well is strongly reduced in the $In_yGa_{1-y}As$ well. Experimental results were found to be in good agreement with numerically obtained dispersion relations and PLE spectra. Although most numerical details were quantitatively covered by the experiments, the predicted Moss-Burstein shift exceeded the observed shift significantly. No consistent interpretation of this effect was found.

ACKNOWLEDGMENT

We would like to thank J. C. M. Henning for many stimulating discussions, and for a careful reading of the manuscript, and R. van Schaijk for his contributions to the software used.

[1] L. Van Hove, Phys. Rev. **89**, 1189 (1953).
[2] See, e.g., F. Bassani and G. Pastori Parravicini, in *Electronic States and Optical Transitions in Solids*, edited by R. A. Ballinger (Pergamon, Oxford, 1975).
[3] H. Chu and Y.-C. Chang, Phys. Rev. B **36**, 2946 (1987).
[4] K. Fujiwara, K. Kawashima, T. Yamamoto, N. Sano, R. Cingolani, H. T. Grahn, and K. Ploog, Phys. Rev. B **49**, 1809 (1994).
[5] H. A. Fertig and S. Das Sarma, Phys. Rev. B **42**, 1448 (1990).
[6] R. W. Winkler, J. P. Kotthaus, and K. Ploog, Phys. Rev. Lett. **62**, 1177 (1989).
[7] D. Weiss, K. von Klitzing, K. Ploog, and G. Weimann, Surf. Sci. **229**, 88 (1990).
[8] L. Smrčka and T. Jungwirth, J. Phys. Condens. Matter **7**, 3721 (1995).
[9] See, e.g., G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructures* (Les Editions de Physique, Les Ulis, 1988), and references therein.
[10] R. K. Hayden, D. K. Maude, L. Eaves, E. C. Valdares, M. Henini, F. W. Sheard, O. H. Hughes, J. C. Portal, and L. Cury, Phys. Rev. Lett. **66**, 1749 (1991).
[11] R. Winkler, Phys. Rev. B **51**, 14 395 (1995).
[12] J. C. Maan, in *Physics and Applications of Quantum Wells and Superlattices*, edited by E. E. Mendez and K. von Klitzing, Vol. 170 of *NATO Advanced Study Institute, Series B: Physics* (Plenum, London, 1987).
[13] L. C. Andreani, A. Pasquarello, and F. Bassani, Phys. Rev. B **36**, 5887 (1987).
[14] M. Potemski, J. C. Maan, A. Fasolino, K. Ploog, and G. Weimann, Phys. Rev. Lett. **63**, 2409 (1989).
[15] F. Ancillotto, A. Fasolino, and J. C. Maan, Phys. Rev. B **38**, 1788 (1988).
[16] A. H. MacDonald and D. S. Ritchie, Phys. Rev. B **33**, 8336 (1986).
[17] E. F. Schubert, *Doping in III-V Semiconductors* (Cambridge University Press, Cambridge, 1993).
[18] See, e.g., C. Weisbuch and B. Vinter, *Quantum Semiconductor Structures* (Academic, London, 1991), Chap. 3.
[19] E. S. Coteles and J. Y. Chi, Phys. Rev. B **37**, 6332 (1988).
[20] M. Sugawara, J. Appl. Phys. **71**, 277 (1992).
[21] M. Kemerink, P. M. Koenraad, P. C. M. Christianen, A. K. Geim, J. C. Maan, J. H. Wolter, and M. Henini, Phys. Rev. B **53**, 10 000 (1996).
[22] J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).
[23] See, e.g., M. Altarelli, in *Heterojunctions and Semiconductor Superlattices*, edited by G. Allan, G. Bastard, N. Boccora, and M. Voos (Springer-Verlag, Berlin, 1986).
[24] M. Guzzi and J. L. Steahly, in *Physics of DX Centers in III-V Ternary Compounds*, edited by J. C. Bourgoin (Trans Tech, Aedermannsdorf, 1989).
[25] C. G. Van de Walle, Phys. Rev. B **39**, 1871 (1989).
[26] K. H. Goetz, D. Bimberg, H. Jürgensen, J. Solders, A. V. Solomonov, G. F. Glinskii, and M. Razeghi, J. Appl. Phys. **54**, 4543 (1983).
[27] R. Cingolani, W. Stolz, and K. Ploog, Phys. Rev. B **40**, 2950 (1989).
[28] J. De-Sheng, Y. Makita, K. Ploog, and H. J. Quesser, J. Appl. Phys. **53**, 999 (1982); B. G. Arnaudov, D. S. Domanevskii, A. M. Issusov, P. L. Gardev, and S. K. Evtimova, Semicond. Sci. Technol. **5**, 620 (1990).
[29] D. G. Deppe, N. D. Gerard, C. J. Pinzone, R. D. Dupuis, and E. F. Schubert, Appl. Phys. Lett. **56**, 315 (1990).
[30] In fact, the usual van Hove condition is fulfilled for almost all transitions at $k=0$, since it only requires equality of the first derivatives of hole and electron dispersions, which are usually zero at the Γ point. However, the resulting effect on the joint density of states is a step of height $m^*/\pi\hbar^2(m^{*-1}=m_e^{-1}+m_h^{-1})$, which is just the density of states of a parabolic band.
[31] L. Gravier, M. Potemski, A. Fisher, and K. Ploog, Solid-State Electron. **40**, 697 (1996).