Quantum-well states under biaxial compression and tension

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Differences in the thermal expansion of a thin GaAs/$Al_xGa_{1-x}As$ multiple-quantum-well (MQW) sample and a thick sample holder to which it is fixed, lead, by varying the temperature, to a homogeneous biaxial strain in the MQW sample. It can be decomposed into a hydrostatic and a uniaxial component. Using different sample holders the stress can be made tensile (quartz) or compressive (BaF_2). In the temperature range between 300 and 20 K we observe in optical transmission the corresponding shift and changing splitting of the exciton lines formed with heavy and light holes. The experimental data are well described by subband calculations based on an 8×8 $\mathbf{k}\cdot\mathbf{p}$ model, which includes the dependence of the band-edge energies on temperature and stress.

I. INTRODUCTION

The application of stress to study near band-edge electron states in semiconductors has recently become important also for quantum-well structures.[1–13] One interesting aspect of these studies is the lifting of the fourfold degeneracy of the topmost bulk valence band due to the symmetry-breaking effect of uniaxial stress and quantum confinement. The splitting of the lowest heavy- and light-hole subbands caused by quantum confinement—and likewise the hole subband dispersion, which is sensitive to it—can be tuned by application of uniaxial stress.[10] So far in experimental and theoretical studies this has been exploited for uniaxial stress in the growth direction[1,10,11] or in the plain[2–4,6–11] of the quantum-well structure. The other interesting aspect is that, while in experiments on bulk material usually only compressive stress is realized, in quantum-well structures it becomes possible to produce also tensile stress either due to lattice mismatch in so-called strained-layer superlattices[14] or by making use of the different thermal contraction of a substrate and a quantum well structure grown on it.[5]

In this communication we present a new method to study the electronic properties of multiple quantum wells (MQW's) under both biaxial compression and tension, which result upon cooling from the different thermal expansion coefficients of a thin GaAs/AlGaAs MQW sample and various sample holders to which it is glued at room temperature. We observe in transmission the lowest light-hole (LH) and heavy-hole (HH) excitons. The spectral position of these excitons and their temperature and stress dependence are in close agreement with subband energy differences calculated from an 8×8 $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian with temperature and stress-dependent band-edge energies.

II. EXPERIMENTAL RESULTS

We have used a structure of 60 GaAs layers of 84.5 Å which are separated by $Al_xGa_{1-x}As$ ($x=0.39$) barriers with a thickness of 230 Å. MQW samples with a dimension of about 3×4 mm^2 are glued on different sample holders by use of a transparent cyanoacrylate adhesive. As sample holders we use BaF_2, ZnSe, and quartz glass. The GaAs substrate (about 200 μm) is then totally removed by selective etching until only the thin MQW structure remains on the sample holder. The etch solution consists of 30% H_2O_2 and an additional amount of NH_4OH to reach a pH value of 7.5. Based on the different thermal expansion coefficients of the MQW structure and the sample holder, we expect considerable strain in the MQW layers, when the samples are cooled down to 20 K. The transmission measurements are performed with the use of a Cary 2300 spectral photometer. The spectral resolution is set to 0.3 nm. The samples are cooled down in a cryostat coupled to a closed-cycle He refrigerator (type RG210 of Leybold Heraeus). By heating the cold head, it is possible to adjust the temperature in the range from 20 to 300 K.

Typical transmission spectra of our samples at 40 K are shown in Figs. 1(a)–1(c). The resonances belong to the lowest light-hole exciton and to the lowest heavy-hole exciton separated by the heavy-hole–light-hole (HH-LH) splitting. The corresponding spectra at room temperature, at which the MQW samples are glued to the sample holders, do not depend on the holder and show two lines

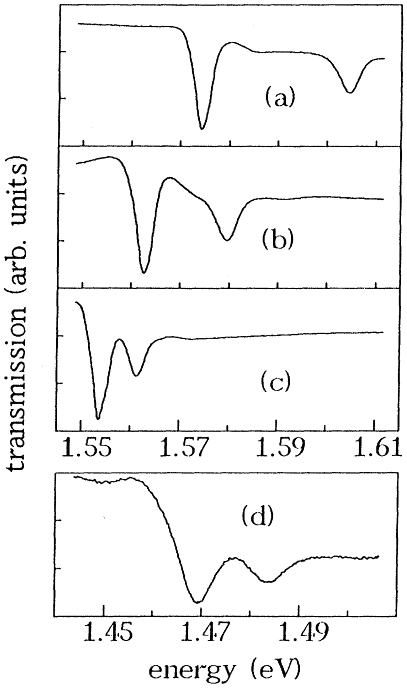

FIG. 1. Transmission spectra of light-hole and heavy-hole excitons for a GaAs/$Al_xGa_{1-x}As$ MQW structure glued on different sample holders. At 40 K (a) BaF_2, (b) ZnSe, (c) quartz glass, and at 293 K (d) ZnSe.

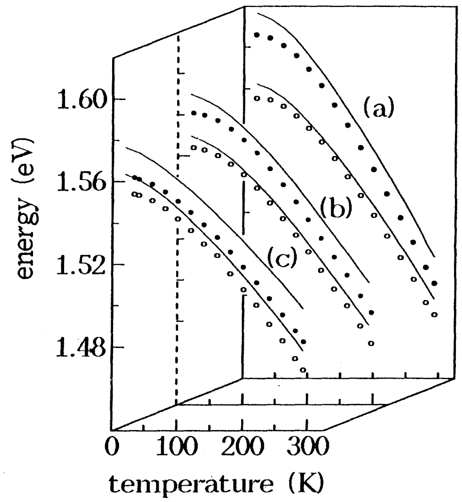

FIG. 2. Spectral position of LH (solid symbols) and HH (open symbols) excitons vs temperature for a GaAs/AlGaAs MQW sample glued on different sample holders. (a) BaF_2; (b) ZnSe; (c) quartz glass. The calculated curves (solid lines) are differences between electron- and hole-subband energies.

at about 1.48 eV split by 17 meV. As an example we show the room-temperature spectrum of the ZnSe sample in Fig. 1(d). Comparing Fig. 1(d) with Figs. 1(a)–1(c) one finds that the lowering of the temperature has two effects: it shifts the average position of the exciton lines to a higher energy and it changes the HH-LH splitting. Both effects depend on the sample holder used. The most striking result of Fig. 1 is the increase of the HH-LH splitting for the sample glued on BaF_2 and its decrease for the sample on quartz, with respect to the confinement splitting observed at room temperature, whereas this splitting is almost independent of the temperature for the sample on ZnSe. An overview of the measured exciton positions versus temperature is given in Fig. 2.

The interpretation of these results is as follows. The general blue shift of the resonances is mainly due to the temperature dependence of the energy gap. Superimposed to this shift, which does not depend on the sample holder, are the effects of the homogeneous biaxial strain induced in the quantum-well plane upon lowering the temperature. Because ZnSe has nearly the same thermal expansion coefficient[15] as the GaAs/$Al_xGa_{1-x}As$ (Refs. 15–17) sample the strain is almost zero and the exciton peaks shift according to the temperature dependence of the GaAs gap energy. The thermal expansion coefficient of BaF_2 (Ref. 18) is about 3 times larger than that of the MQW sample. Thus, by lowering the temperature, the faster reduction of the lattice parameter of BaF_2 results in a biaxial compression of the MQW sample. For the sample, one gets biaxial tension. We can produce compressive stress of up to 0.3 GPa using BaF_2 as sample holder and tension of -0.12 GPa with quartz glass as sample holder. The biaxial strain in the MQW plain, which is determined by the difference of the thermal expansion coefficients of the MQW sample and the sample holder, can be decomposed into a hydrostatic and a uniaxial component in the growth direction. While the hydrostatic component contributes to the shift of the average spectral position of the quantum-well excitons, the uniaxial component is responsible for the observed changes in the HH-LH splitting. From the numerical values of the thermal expansion coefficients the effects are expected to be about 3 times stronger for BaF_2 than for quartz as a sample holder.

III. THEORY

In order to confirm this interpretation of our results we have performed subband calculations based on an 8×8 $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian with temperature and stress-dependent band-edge energies. From literature[16,17] we take the temperature dependence of the gap energy for the well (GaAs)

$$E_0^W(T)=\left[1.519-5.408\times10^{-4}\frac{T^2}{T+204}\right]\text{eV} \quad (1)$$

and for the barrier material ($Al_{0.39}Ga_{0.61}As$)

$$E_0^B(T)=(2.039-4.41\times10^{-4}T)\ \text{eV} . \quad (2)$$

The change of the gap difference $E_0^B(T)-E_0^W(T)$ is distributed according to the 65/35 rule to the conduction valence-band offset.

The biaxial stress S induced in the x-y plane of the MQW is given by

$$S = e_{xx}(c_{11}+c_{12}) + e_{zz}c_{12} \tag{3}$$

while there is zero stress in the growth direction

$$0 = 2e_{xx}c_{12} + e_{zz}c_{11} \; . \tag{4}$$

Decomposition of the strain tensor into hydrostatic and uniaxial part gives

$$e_{xx} = e_{yy} = e_{zz}^{H} = \frac{c_{11}}{c_{11}^2 + c_{11}c_{12} - 2c_{12}^2} S \tag{5}$$

and

$$e_{zz}^{\mathrm{uni}} = \frac{c_{11}+2c_{12}}{-c_{11}^2 - c_{11}c_{12} + 2c_{12}^2} S \; . \tag{6}$$

The biaxial stress S can be obtained with $e_{zz}^{H} = \Delta l / l$ from Eq. (5), where Δl is the difference between the lattice parameter of the free sample at temperature T and its value for the fixed sample at the same temperature, which is determined by the thermal contraction of the holder between room temperature and T. The temperature dependence of the linear thermal expansion coefficients α_i (i = MQW, holder) requires to formulate $\Delta l / l$ as the integral expression

$$\frac{\Delta l}{l} = \int_{293\,\mathrm{K}}^{T} [\alpha_{\mathrm{MQW}}(T) - \alpha_{\mathrm{holder}}(T)] dT \; . \tag{7}$$

Eliminating the biaxial stress S from Eq. (6) we can express the uniaxial strain component as

$$e_{zz}^{\mathrm{uni}} = -\frac{c_{11}+2c_{12}}{c_{11}} \frac{\Delta l}{l} \; . \tag{8}$$

The variation of the conduction-band edge with strain is

$$\Delta E_c = 2a' \frac{c_{11}-c_{12}}{c_{11}} \frac{\Delta l}{l} \tag{9}$$

while for the valence band we obtain

$$\Delta E_v = \left[2a'' \frac{c_{11}-c_{12}}{c_{11}} \pm b \frac{c_{11}+2c_{12}}{c_{11}} \right] \frac{\Delta l}{l} \; . \tag{10}$$

Equations (9) and (10) have to be evaluated for well and barrier material, which differ in their deformation potentials (a', a'' and b) and compliance constants c_{ij} which are assumed independent of T. Note, that we consider the hydrostatic shift of conduction and valence bands separately. For GaAs we use the screened hydrostatic deformation potential $a'' = -1.6$ eV of Ref. 20 and $a' - a'' = -8.4$ eV as experimental value of the interband deformation potential,[16] the values for the barrier material are taken from Ref. 17. The plus (minus) sign in Eq. (10) refers to the heavy (light) hole.

The energies of electron and hole subbands were calculated from a multiband Hamiltonian using the concept outlined in Ref. 21. This method is particularly useful for a piecewise constant potential as in the present case and is not restricted to simplified (parabolic) dispersion relations of conduction and valence bands. We use an 8×8 $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian which includes exactly the coupling between the Γ_6 conduction band and the spin-orbit-split valence bands $\Gamma_8 + \Gamma_7$ and considers remote bands by second-order perturbation theory.[22] Temperature and stress-dependent band-edge energies as described before are used. Because the band-edge parameters of the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian are known for well (GaAs) and barrier material (AlGaAs), as are the elastic constants, deformation potentials, and linear thermal expansion coefficients,[15–19] the calculations are free of any fitting parameter.

IV. DISCUSSION

In Fig. 2 we compare the temperature dependence of the observed spectral position of the lowest heavy- and light-hole excitons with the calculated transition energies (solid lines in Fig. 2). The overall trends of the experimental results are well described by the calculated data. In the case of ZnSe [curve (b) of Fig. 2] the shift of the spectral positions of the heavy- and light-hole transitions is determined mainly by the temperature dependence of the energy gaps given by Eqs. (1) and (2). In addition to this shift the data for BaF_2 [curve (a)] and quartz [curve (c)] show the shift of the resonances and the change of the HH-LH splitting due to the hydrostatic and uniaxial components of the biaxial strain, respectively. In detail, the theoretical values are at about 10 meV higher energies than the experimental data, which corresponds to the binding energy of the lowest excitons in a quantum well of this width.[23] The calculated splitting of the transitions connected with heavy- and light-hole subbands is somewhat larger than in experiment.

The different effects of biaxial compression and tension, in particular of their hydrostatic and uniaxial components, are shown in Figs. 3 and 4, respectively. The hydrostatic stress component shifts the average spectral position of heavy- and light- hole exciton for the MQW sample on BaF_2 [curve (a) in Fig. 3] and on quartz [curve (c)] with respect to that of the ZnSe sample [curve (b)], which is almost free of strain. Hydrostatic compression ($\Delta l < 0$, as for the MQW sample on the BaF_2 holder) and negative hydrostatic interband deformation potential $a' - a''$ increase the gap [see Eqs. (9) and (10)] and likewise the average spectral position of the observed excitons, while hydrostatic tension ($\Delta l > 0$ for MQW on quartz) decreases it. The calculated values (Fig. 3, solid lines) are in good agreement with the experimental data. On the other hand, the uniaxial stress component connected with a biaxial compression (tension) is tensile (compressive) as can be seen from Eq. (8). Consequently the HH-LH splitting resulting from the quantum confinement at room temperature is increased (decreased) for the BaF_2 (quartz) sample [Fig. 4 and Eq. (10)]. Note that the theoretical values in Fig. 4 are shifted by about 5 meV with respect to the experimental data. This shift can be ascribed only partially to the difference in the exciton binding energies of heavy- and light-hole excitons.[23,24] As a general comment on the theoretical data we should mention that the shift of the band edges as discussed above is, in fact, much more important than the change in the confinement energies connected with it.

In conclusion, our study demonstrates the possibility to investigate the effets of biaxial compression and ten-

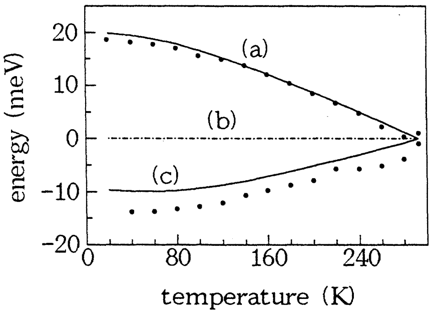

FIG. 3. Temperature shift of the average spectral position of LH and HH exciton transitions for MQW on (a) BaF_2 and (c) quartz glass with respect to that for MQW on (b) ZnSe in comparison with calculated values (solid lines).

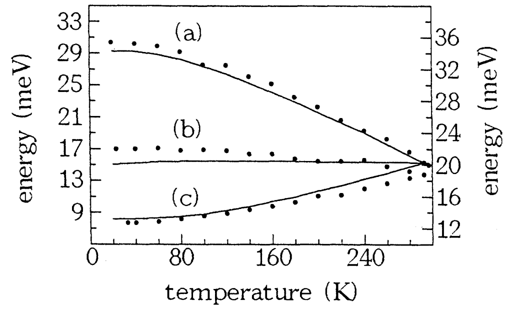

FIG. 4. Splitting of the LH and HH excitons for MQW on (a) BaF_2, (b) ZnSe, and (c) quartz glass vs temperature in comparison with calculated values (solid lines).

sion on quantum-well states by exploiting the different thermal expansion of the MQW sample and properly chosen sample holders to which it is glued. The observed spectral positions of the lowest heavy- and light-hole excitons are well described by subband energy differences calculated from a multiband effective-mass Hamiltonian with temperature- and stress-dependent band-edge energies. As possible extensions of this work we would like to mention the study of transitions connected with higher subbands and of inhomogeneous biaxial strain using, e.g., $CaCO_3$ as a sample holer.

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