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Light and heavy valence subband reversal in GaSb-AlSb superlattices

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We report optical-absorption measurements in high-quality GaSb-AlSb superlattices. The spectra exhibit the two-dimensional density of states and free-exciton peaks. The effect of strain induced by the lattice mismatch is manifested by the anomalous energies of the absorption edges and the reversal of the heavy- and light-hole exciton positions. The data are in good agreement with a simple effective-mass theory.

A variety of superlattices (SL) built with two different semiconductors have been achieved by molecular-beam epitaxy (MBE) or metal-organic chemical vapor deposition. They exhibit structural as well as optical and transport properties indicating a high crystalline quality, which implies that the small but generally nonzero lattice mismatch of the hosts is accomodated by elastic deformations. Recently, successful growth and characterization of SL's made from materials with deliberately large lattice mismatches ($\delta a/a \sim 1\%$) have been reported. However, most of the effort has been focused[1] on systems in which the small gap material is a ternary alloy, namely, GaP-GaAs$_x$P$_{1-x}$ (Ref. 2) and GaAs-In$_x$Ga$_{1-x}$As (Refs. 3 and 4). This makes precise analysis of the situation difficult as it requires an accurate knowledge of many physical parameters in the alloys, which are generally unavailable. For a quantitative evaluation of the important strain effects, the binary system of GaSb-AlSb with a mismatch of 0.65% is clearly a good candidate which has recently been fabricated by MBE.[5] Preliminary optical-absorption[6,7] and luminescence[7-9] data have been reported, indicative of a strain-induced shrinkage of the GaSb band gap.[6] We present here optical-absorption measurements performed at low temperatures in high-quality GaSb-AlSb SL's. The absorption spectra exhibit well-defined free-exciton peaks separated by plateaus reflecting the two-dimensional density of states. The shrinkage of the GaSb band gap is accompanied by a remarkable reversal of the heavy- and light-hole subbands, an effect hitherto unobserved in SL's.

Our structures were grown on (100) semi-insulating GaAs substrates, with the following growth sequence: a 1000-Å-thick GaAs smoothing layer, a 3000-Å-thick AlSb layer, n periods of alternating layers of GaSb and AlSb with thicknesses d_1 and d_2, respectively, and a 200-Å thick GaSb protective layer. The layers are of high purity, with an impurity concentration in the 10^{15} cm^{-3} range. The structures were evaluated from x-ray measurements with an automated diffractometer,[10] using the Cu-$K\alpha$ radiation and the (111) planes of Ge for monochromating and collimating the incident beam. Figure 1 shows the standard intensity versus angle plot of the (004) diffraction patterns on a logarithmic scale for the two samples reported here ($S1$ and $S2$). It is seen that a large number of high-order satellite peaks are resolved. While the orders cannot be precisely assigned,

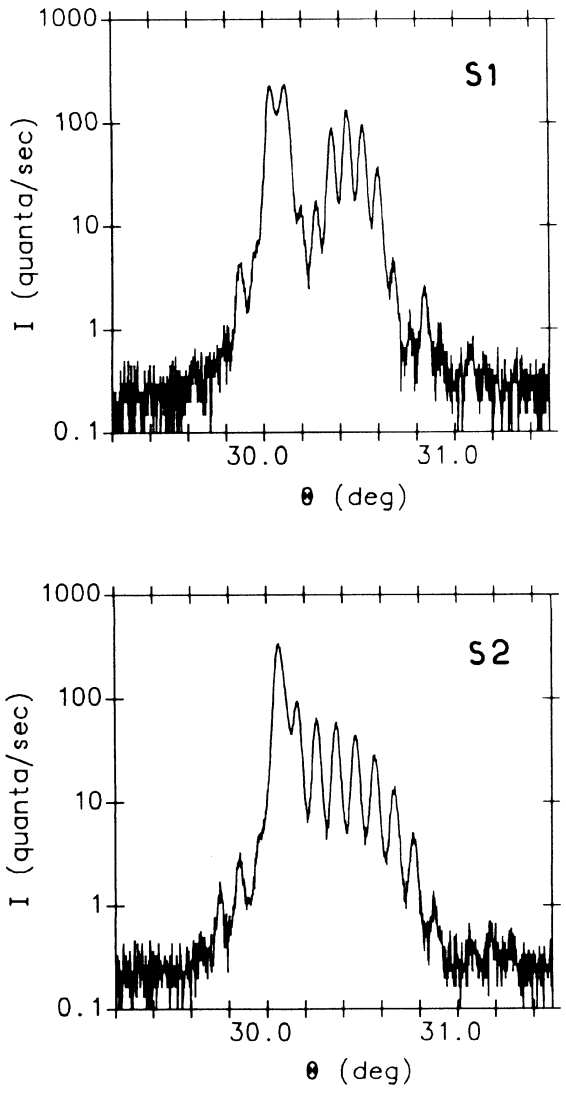

FIG. 1. Cu-$K\alpha_1$ (004) diffraction patterns of GaSb-AlSb superlattices: $S1$ (upper), 181–452 Å; $S2$ (lower), 84–419 Å.

partly because of contributions from the buffer and the protective layer, their presence and their narrow peak width demonstrate the high structural quality of the samples. In addition, the period can be accurately determined, (632.8 ± 1) Å for $S1$ and (502.8 ± 1) Å for $S2$, corresponding to d_1 (GaSb) = 181 Å, d_2 (AlSb) = 452 Å and $d_1 = 84$ Å, $d_2 = 419$ Å, respectively. The number of periods is $n = 10$ for both samples.

Optical-transmission spectra were measured using a single-beam setup and compared to the transmission spectrum of a bare semi-insulating GaAs substrate as described in Ref. 6. Figure 2 shows the observed spectra which exhibit clearly the steplike behavior characteristic of the two-dimensional density of states, and also exciton absorption peaks at the onset of the steps. The excitonic features are indicative of the high quality of these structures and of the type-I nature of this system, i.e., both conduction and valence states are confined in the GaSb quantum wells. The transmission spectrum of $S1$ presents two unusual features: (i) the B exciton peak, which, in view of its intensity, is likely to involve the heavy-hole subband H_1 and the ground-conduction subband E_1 occurs at 810 meV. In a simple quantum-well model, the sum $H_1 + E_1$ of the corresponding confinement energies is easily estimated to be 25 meV, so that this transition is expected to occur at $E_g^{\mathrm{GaSb}} + 25$ meV = 835 meV. The observed energy position is interpreted in terms of a strain-induced GaSb band-gap shrinkage. The same effect, in fact, is seen on the transmission spectrum of $S2$ for which $H_1 + E_1 = 90$ meV. The first exciton peak in this sample is observed at 870 meV, about 30 meV below the predicted value without strain. (ii) A well-resolved structure A is observed 20 meV below the B exciton peak, with an absorption coefficient somewhat smaller but in the same range of magnitude. As will be discussed below, this structure corresponds to absorption by a free exciton involving the first light-hole level h_1. As a striking consequence of the strain, the ground light-hole state becomes the ground valence state of the system.

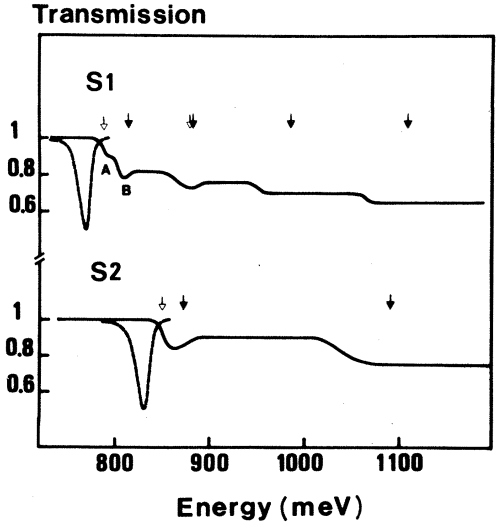

FIG. 2. Transmission (full line) and luminescence (dashed line) spectra of the two GaSb-AlSb superlattices ($S1$,$S2$). The solid (open) arrows indicate the calculated transition energies involving the heavy-hole (light-hole) states as discussed in the text. The band gap of bulk GaSb is 810 meV.

The interpretation of these data is based on the following theoretical considerations.[11] The lattice constants of GaSb and AlSb at 300 K are $a_1 = 6.0959$ Å and $a_2 = 6.1355$ Å, respectively. The lattice mismatch, $\delta a/a = 0.65\%$, will retain essentially the same value at low temperature, as can be seen from a comparison of the thermal expansion coefficients.[12] In the SL, the GaSb layers stretch in the x,y directions of the layer plane, as a result of a biaxial tensil stress, while the AlSb layers are under equal compressive biaxial stress. This situation can be analyzed in terms of the sum of a hydrostatic dilatation (or compression) plus a uniaxial compression (or dilatation) in the (100) z direction of the GaSb layers (or AlSb layers). As the elastic constants of GaSb and AlSb are essentially the same, the in-plane lattice parameter of the strained layers $a_\perp$ is simply given by

$$a_\perp (d_1 + d_2) = a_1 d_1 + a_2 d_2 \ . \tag{1}$$

The strength of the stress X exerted on the GaSb layers can be expressed in terms of the usual elastic constants K and μ equal[13] to 5.64×10^{10} and 2.16×10^{10} (MKS units), respectively,

$$X = \left(\frac{2}{9K} + \frac{1}{6\mu} \right)^{-1} (a_\perp - a_1)/a_\perp \ . \tag{2}$$

This stress gives rise to the following modification[14] of the GaSb band parameters: (i) a shrinkage of the GaSb band gap due to the hydrostatic dilation of strength X; and (ii) an increase of the GaSb band gap and a splitting of the Γ_8 valence band due to the uniaxial compression of strength X in the z direction. This results in a fundamental light hole to conduction band gap,

$$E_c - E_h = E_g^{\mathrm{GaSb}} - 2a(S_{11} + 2S_{12})X - b(S_{11} - S_{12})X \ , \tag{3}$$

and a larger heavy hole to conduction band gap

$$E_c - E_H = E_g^{\mathrm{GaSb}} - 2a(S_{11} + 2S_{12})X + b(S_{11} - S_{12})X \ . \tag{4}$$

Here, a and b are the deformation potentials and S_{11}, S_{12} are the elastic compliance constants. For GaSb,[15]

$$\delta E_g / \delta p = 3a(S_{11} + 2S_{12}) = 14.27 \times 10^{-11} \ \mathrm{eV\,N^{-1}\,m^2}$$

and

$$2b(S_{11} - S_{12}) = 8.4 \times 10^{-11} \ \mathrm{eV\,N^{-1}\,m^2} \ .$$

E_c, E_H, and E_h refer to the positions of the $|S_{1/2}\rangle$ (conduction), $|P_{3/2}\rangle$, and $|P_{1/2}\rangle$ (valence) band edges, respectively.

Thus the SL ground valence state may be a light-hole state, despite its larger confinement energy. On the other hand, the AlSb layers present an increased fundamental heavy hole to conduction band gap and a slightly larger light hole to conduction band gap. In the following, we neglect the modifications in the AlSb band structure for they will not change the results significantly, particularly because the AlSb layers are much thicker and, consequently less strained than the GaSb layers. Now, since the spin-orbit splitting $\Delta = 752$ meV is large compared with the strain effects, we can consider that the superpotential arising from the electron affinity and band-gap difference between the two host materials commutes with the strain Hamiltonian. In this case, the $J_z = \pm \frac{3}{2}$ (heavy hole) and $J_z = \pm \frac{1}{2}$ (light hole)

states remain eigenstates of the total Hamiltonian, as long as $\vec{k}_\perp = (k_x, k_y) = 0$. Then we can calculate the SL eigenenergies E_i, h_i, H_i within the envelope wave function formalism,[16] using for the light hole and conduction states the modified value of the GaSb band gap and assuming a given value for the light-hole valence-band offset ΔE_v^h, and a smaller value for the heavy-hole valence-band offset $\Delta E_v^H = \Delta E_v^h - 2b(S_{11} - S_{12})X$. From absporption coefficient strength considerations,[6] only the Γ extrema of the host band structure are to be considered. We use Kane's three-bands model[17] because Δ is not large as compared to the band gaps, which are 2200 and 810 meV for AlSb and GaSb, respectively. We take $m^* = 0.041 m_0$ for the GaSb band-edge conduction mass, and $m_H = 0.33 m_0$ for the heavy-hole masses in both materials.

In $S1$, the lattice mismatch obtained from Eq. (1) is 0.46%, so that $E_h - E_H = 32$ meV. In this sample, we observe four transitions involving heavy holes, as seen in Fig. 2. This implies that there are at least four bound heavy-hole levels in the GaSb quantum well, which leads to $\Delta E_v^H \gtrsim 40$ meV and $\Delta E_v^h \gtrsim 70$ meV. Using these values, we get two bound light-hole levels. Assuming the natural-parity-selection rule,[18] the calculated transition energies are $H_1 \rightarrow E_1 = 815$ meV, $H_2 \rightarrow E_2 = 884.5$ meV, $H_3 \rightarrow E_3 = 987$ meV, $H_4 \rightarrow E_4 = 1112$ meV (solid arrows in Fig. 2), and $h_1 \rightarrow E_1 = 790$ meV, $h_2 \rightarrow E_2 = 881$ meV (open arrows in Fig. 2). The calculated transitions towards E_1 are thus in very good agreement with the A and B peaks, and the transitions towards E_2 both contribute to the third experimental peak. These results evidence the predicted reversal of the light- and heavy-hole levels. Had $\Delta E_v^h = 90$ meV been used, for instance, a third bound light-hole level would have appeared, corresponding to $h_3 \rightarrow E_3$, at 1029 meV, which is not observed experimentally. More generally, further increase of the valence-band offset does not affect significantly the quantitative agreement for the observed transitions, but leads to the prediction of additional $h_i \rightarrow E_i$ $(i > 3)$ transitions which are not observed. Keeping $\Delta E_v^H = 40$ meV and taking $\Delta E_v^h = 80$ meV to account for the lattice mismatch [Eq. (1)], we find that in $S2$ $h_1 \rightarrow E_1 = 850$ meV and $H_1 \rightarrow E_1 = 873$ meV. Both energies are within the linewidth of the observed exciton peak and, as already pointed out, are significantly smaller than the expected values without strain. Besides, $H_2 \rightarrow E_2 = 1092$ meV is in reasonable agreement with experiment. Increasing ΔE_v^h up to 100 meV in this case would result in the prediction of an unobserved $h_2 \rightarrow E_2$ transition at 1123 meV.

Finally, we wish to discuss briefly the strength of the absorption coefficient in these structures. As pointed out in Ref. 6, the magnitude of the observed absorption coefficient on the absorption plateaus is in agreement with the theoretical value. The latter is proportional to an optical-matrix element between the atomic part of the wave functions, which is three times larger for transitions involving a heavy hole than for those involving a light hole. It is also proportional to the electron-hole reduced mass, which raises the problem of the intricate kinematics of the various hole subbands with respect to the in-layer motion. The $k_\perp$ dispersion relations of the H_i and h_i valence subbands are not readily attainable without complex computation.[19] However, when h_1 and H_1 are well separated in energy, we may argue that the hole masses are largely governed by the effect of strain, which is known[20] to exchange the light and heavy masses perpendicular to the direction z. Then the reduced mass involving the "light" hole should be about twice that corresponding to the "heavy" hole, and the ratio of the corresponding absorption coefficients should be $\frac{2}{3}$, in agreement with the relative strengths of the A and B transitions in $S1$. If the heavy- and light-hole masses were not exchanged, this ratio would be equal to $\frac{1}{6}$ which is far too small.

Figure 2 also shows luminescence spectra (dashed lines) obtained in our SL's. They all lie 30 to 50 meV below the observed exciton absorption transitions. This indicates that these spectra correspond to extrinsic radiative recombination phenomena (most probably band to acceptor recombination) that are beyond our interest in this work.

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