Pressure Dependence of Band Offsets in an InAs-GaSb Superlattice

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Using magneto-optical methods, we have measured the pressure dependence of the energy difference between subbands in an InAs-GaSb superlattice associated with the GaSb valence and the InAs conduction bands, respectively. The experimental results allow a determination of the pressure dependence of the energy separation between the InAs conduction band and the GaSb valence band which is found to decrease at a rate of 5.8 meV/kbar. This result shows that both the conduction- and the valence-band offsets are pressure dependent. Therefore these experiments constitute a critical test for different theories of band lineup.

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Usually, the relative positions of the energy bands within a single bulk semiconductor are well known. However, the positions of the band edges in one semiconductor relative to those in another when they are in contact with each other (band lineup) provide a problem in solid-state physics which is neither experimentally nor theoretically well understood. Yet this problem has become particularly relevant, and at the same time experimentally accessible, through the possibility of the growth of high-quality interfaces and heterojunctions by modern growth techniques like molecular-beam epitaxy (MBE).[1,2]

Conceptually the band-lineup problem can be divided into two parts: (i) Which energy level must be lined up at the interface in order to determine the band offsets, and (ii) where does this level lie with respect to the band edges? There exist several band-lineup theories, but the accuracy of both experimental and theoretical values is not sufficient to distinguish clearly between them. The essential difference between these theories is their choice of this energy level. As hydrostatic pressure has a strong effect on the relative positions of the energy bands in a solid, and therefore in general on the positions of the bands with respect to this common energy, it is of considerable importance to investigate the band lineup in a semiconductor interface as a function of pressure and to compare the results with existing band-lineup models. For this purpose we present experimental results of the pressure dependence of the lineup of the bands at the InAs-GaSb interface, by use of magneto-optical methods.

We have chosen the InAs-GaSb interface because it has been studied experimentally very carefully before[3-6] and because this system provides one of the most severe tests for any band-lineup theory. The peculiarity of this system is that the conduction-band (CB) edge of InAs is at a lower energy than the valence-band (VB) edge of

GaSb. This fact leads to a strong dependence of the electronic properties of InAs-GaSb heterostructures, e.g., superlattices (periodic alternate thin GaSb and InAs layers), on the exact value of this energy overlap. Several results of optical experiments on this system can be explained with a value of 150 meV for this difference, with an experimental error of 50 meV.[4-6] These experimental values are probably the most accurately known in the literature; note that, for instance, the lineup of the most extensively studied GaAs-Ga$_{1-x}$Al$_x$As system is still controversial.[7] Hydrostatic pressure has a strong effect on the energies of the bands in these semiconductors. The energy gap, E_G, increases by 10 meV/kbar and 14 meV/kbar for InAs and GaSb, respectively.[8] In particular, at easily attainable pressures (10 kbar), the band-gap variation is comparable to the energy overlap between the valence and the conduction bands.

The main features of the electronic band structure of the investigated superlattice (consisting of many layers of alternate 12-nm InAs and 8-nm GaSb, grown on a GaSb ⟨100⟩ substrate) is illustrated in Fig. 1. This superlattice shows an electronlike level (E_1, at higher energy than the InAs bulk CB edge because of the confinement in the InAs layer) and a holelike level (H_1, at a lower energy than the GaSb VB edge because of the confinement in the GaSb layer). An extensive review of the electronic properties of this kind of superlattices can be found in Ref. 6. In a simplified manner, appropriate for the understanding of the present experiments, the energy difference between the E_1 and the H_1 subband edge at zero wave vector is given by the InAs-CB GaSb-VB discontinuity Δ minus the confinement energy for the electrons (the shift of the subband with respect to the InAs band edge) minus the hole confinement energy. Therefore a measurement of $E_1 - H_1$ as a function of pressure provides direct information about the pressure dependence of the band lineup. Previous measure-
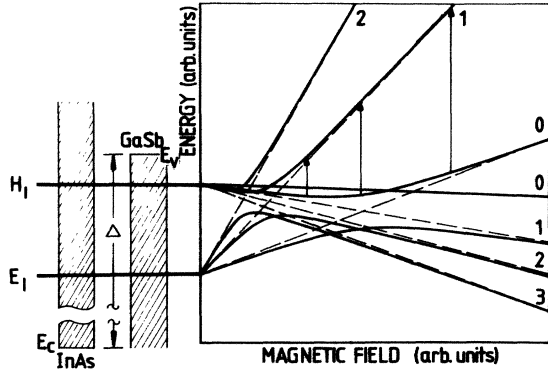
FIG. 1. One period of an InAs-GaSb superlattice showing the band lineup of the InAs conduction- and the GaSb valence-band edges, and the positions of the electronlike subband (E_1) and the holelike subband (H_1). In the right-hand part of the figure the holelike (moving downward) and electronlike (moving upward) Landau levels of these subbands in the absence of (dashed lines) and in the presence of (solid lines) coupling between them for a magnetic field perpendicular to the layers of the superlattice are shown schematically. The arrows indicate transitions which have been observed experimentally. Because of the coupling between the electronlike and holelike Landau levels these transitions have an interband character in the vicinity of, and an intraband (cyclotron resonance) character further away from, the crossing.

ments[4,5] on the same sample by use of far-infrared magneto-optical transmission at zero pressure have determined E_1 to be 40 meV lower than H_1, and subsequent theoretical calculations[9] have shown that these experiments can be explained with band-structure calculations using a value of 150 meV for Δ. Here we report the results of the same experiment, i.e., measurement of $E_1 - H_1$ by use of far-infrared absorption in a magnetic field, for different hydrostatic pressures. This is illustrated in Fig. 1, which shows schematically the holelike and the electronlike Landau levels of the sample as a function of a magnetic field perpendicular to the layer. As usual, the continuum of states for motion in the plane of the layer is split into a set of equidistant linearly field-dependent levels, with hole levels moving downward and electron levels moving upward in energy. However, a small interaction between the holelike and the electronlike Landau levels leads to an anticrossing between the two as indicated in the figure. Transitions which can be observed in the present experiment are also shown. The experiments were done at $T = 4.2$ K in a commercial Cu-Be liquid pressure cell, with mineral oil as the pressure-transferring medium (see Ref. 8, p. 184). An optically pumped cw molecular gas laser was used as radiation source.

Representative transmission curves at different radiation energies as a function of the magnetic field at fixed pressure and a plot of the observed transmission minima as a function of radiation energy are shown in Fig. 2. If,
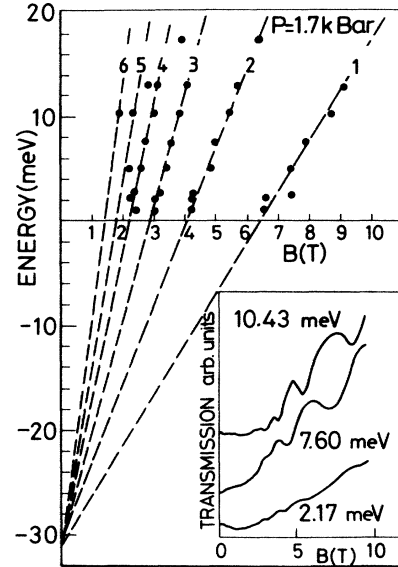

FIG. 2. Observed transition energy between subbands of an InAs-GaSb superlattice as a function of magnetic field at a pressure of 1.7 kbar. The inset shows the experimental spectra. The dashed lines show the linear extrapolation (i.e., with the assumption of pure interband transitions) indicating a material with a negative energy gap $E_1 - H_1$. The transitions are labeled according to the noninteracting model in which the quantum number is that of the two participating Landau states.

in a qualitative way, one assumes unperturbed, equidistant, linearly field-dependent Landau levels (no anticrossing), a linear extrapolation to zero field (the dashed lines) leads to a negative energy gap, i.e., $E_1 - H_1$. In this way the applied magnetic field is used to obtain the zero-field properties of the sample. Figure 3 shows the pressure dependence of the last high-field transition of
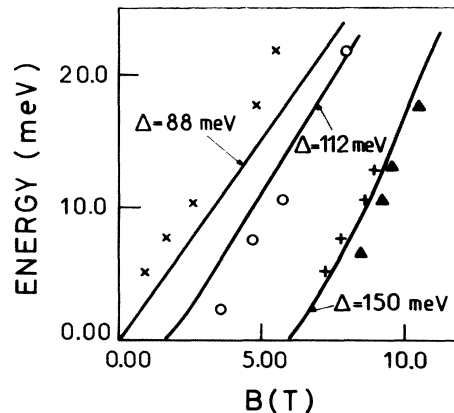

FIG. 3. Pressure dependence of the high-field transition at (triangles) 0, (plusses) 1.7, (circles) 6.6, and (crosses) 10.7 kbar in an InAs-GaSb superlattice. The lines are theoretical calculations of these transitions, with assumption of a linear pressure dependence of the band-lineup parameter Δ.

Fig. 2 with increasing pressure. This transition moves to lower magnetic fields, while at the same time the slope of the energy-versus-field dependence decreases by 30%. These results are a direct consequence of the pressure dependence of the lineup at the interface: If the energy difference between the GaSb VB and the InAs CB decreases, the energy separation between the E_1 and the H_1 subbands will also decrease. If we assume no interaction between the hole and electronlike Landau levels (i.e., simple interband Landau-level transitions obeying the selection rule $\Delta n = 0$, no anticrossing), the data can be analyzed by the drawing of straight lines through the transitions as shown in Fig. 2 and evaluation of the intercept with the energy scale at zero field as $E_1 - H_1$ at a given pressure. In this way, one finds that this quantity decreases linearly with pressure at roughly 4 meV/kbar. Obviously such a simplified analysis disregards the coupling between the energy levels and, in particular, does not explain the change of slope which is observed. As can be seen from Fig. 1, inclusion of the coupling between the levels has two effects. First, as $E_1 - H_1$ decreases with increasing pressure, the transitions at a fixed energy (i.e., $0 \rightarrow 1$, as indicated in the figure) move to lower magnetic field, and second, the field at which anticrossing occurs decreases. This latter effect results in a gradual change in character of this particular transition, i.e., a changeover from a more interbandlike transition with a steeper slope to a more intrabandlike (cyclotron resonance) transition with a lesser slope. To analyze this subtle band-structure behavior in more detail, we calculate the pressure dependence of the full band structure within the framework of a six-band $\mathbf{k} \cdot \mathbf{p}$ model as described elsewhere.[9] In the calculation, the full VB-CB coupling is taken into account, both within each material and between the adjacent unstrained materials, by use of proper boundary conditions for the wave functions at the interface. Standard values for the band parameters are used and the only adjustable variable is Δ which is assumed to be linearly pressure dependent. The results are shown in Fig. 3 as the lines. The best agreement with the experiments is obtained by use of a decrease of Δ of 5.8 meV/kbar. This slightly stronger pressure dependence is obviously a consequence of the inclusion of all other effects of the band structure neglected in the more simple analysis (nonparabolicity, subband coupling, effects of this coupling on the confinement energies, etc.). The calculation also shows the tendency of the slope to decrease with pressure as experimentally observed. The essential experimental result therefore is that the offset between the InAs CB and the GaSb VB reduces at a rate of 5.8 meV/kbar. Note that because of a slight lattice mismatch between GaSb and InAs, the band offset one measures in superlattice experiments will be affected by strain.[10-12] However, since the compressibilities of InAs

and GaSb are nearly equal,[8] no additional strain is induced by the pressure, and hence the pressure dependence of the offset is not affected.

As the InAs and GaSb energy gaps increase by 10 meV/kbar and 14 meV/kbar, respectively, it is therefore clear that our experimental results imply that if the pressure is increased, neither the valence bands (which would lead to a decrease of Δ of 10 meV/kbar) nor the conduction bands (which similarly give 14 meV/kbar) in both materials remain constant. It is evident that if the criterion which determines the band offset is the lineup of a reference level, this will be the same for all pressures. The position of the energy bands with respect to that level, however, will in general be pressure dependent. Band-lineup models should be able to explain consistently this pressure dependence of the bands and the band offsets. In this connection we will briefly discuss different theoretical approaches. The most recent suggestion, proposed by Langer and Heinrich,[13] derives the valence-band offsets by use of transition-metal impurity levels as the common energy. To be consistent with our experimental results the position of these deep-level impurities must show a pressure dependence with respect to both the VB and the CB. For GaAs this is indeed so (the Cr level increases by 4.8 meV/kbar with respect to the VB.[14] Unfortunately, in InAs and GaSb deep-level impurity levels are not studied in sufficient detail to make a more quantitative statement. If, as recently postulated,[15,16] the charge-neutrality level is used as the reference energy, the pressure dependence can be estimated crudely from the work of Tersoff[16] by the assumption that the relative position of this level in the energy gap is not pressure dependent. This estimate gives 2 meV/kbar for Δ, which is close to the experiment result. It should be noted that the pioneering Harrison[17] model, which measures the position of the valence bands relative to the average atomic potential in the semiconductors, would predict that Δ varies as the InAs gap (the relative positions of the valence bands being almost pressure independent), which is not in agreement with the experiment. From other methods, such as the electron affinity rule,[18] the theory by Frensley and Kroemer,[19] and *ab initio* calculations,[20] it is rather difficult to extract predictions about the pressure dependence of the band lineup.

In summary, we have measured the pressure dependence of the InAs-GaSb band lineup. Our data show that offset between the GaSb VB and the InAs CB decreases by 5.8 meV/kbar. This value cannot be explained by the pressure dependence of the energy gaps in the bulk materials alone. In addition, the experiments show a pressure-dependent gradual change from interband to intraband transitions, effects which can be explained by our taking into account the full band structure of the system. We believe that the study of the pressure dependence of the band offset may be a useful

tool for the test of heterojunction lineup theories, the main point being that since the band structure of each material at the interface is strongly pressure dependent, the comparison of the band offsets with and without pressure is in some sense equivalent to a comparison of different samples.

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