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LETTER TO THE EDITOR

Orientation and pressure dependence of the band overlap in InAs/GaSb structures

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Abstract. The band overlap at the InAs/GaSb interface has been measured using electron and hole densities deduced from magnetotransport measurements, combined with self-consistent energy level calculations, for structures with both [001] and [111]A orientations. This band crossing is found to be 140 meV for the [001] orientation but increases to 200 meV for [111]A. The difference is attributed to the presence of an interface dipole for [111]A growth. In addition, the band overlap decreases, with applied hydrostatic pressure, at a higher rate for the [111]A orientation.

When an interface is formed between two semiconductors it is of fundamental importance to know how the band edges in one material line up relative to those in the other [1]. There has been a lot of interest in band offsets, both in their experimental measurement by several different methods and in the many suggested theoretical models that may be used to predict the offsets in new systems. An important question in this is the role of the interface layer itself. III–V semiconductors crystallize in the zinc-blende structure. The [001] and [111] directions have substantially different atomic arrangements at the interfaces between the materials. For both growth directions atomic planes of cations alternate with those of anions. Along the [001] direction the atomic planes are equally spaced and are joined by bonds inclined at 54.7° to the [001] axis. For the [111] direction the planes are alternately connected by bonds parallel to the [111] direction and three times as many bonds inclined at 70.5° to that direction. This results in an asymmetry in the local environment at a [111] interface, leading to the possible formation of a large dipole moment which will influence the band offsets. In this letter we demonstrate, using InAs/GaSb, that the band alignment is strongly orientation dependent. Such an orientation dependence of the band offset has already been reported for thin surface layers of Ge on GaAs [2], but no such effect has previously been reported in electrically or optically active heterostructures. Furthermore, the band overlap is found to change at a different rate with hydrostatic pressure for these two orientations.

InAs/GaSb is a type II system with a large band offset leading to an overlapping of the conduction band edge of InAs and the valence band edge of GaSb. For an InAs layer thickness in excess of 85 Å, the system is said to be semimetallic, and charge transfer occurs between the layers, leading to a two-dimensional electron gas in the InAs layers and a two-dimensional hole gas in the GaSb layers [3]. Real samples are not in fact totally intrinsic; the electron concentration is often larger than that of the holes. The difference is attributed to the presence of donor interface defects [4] and pinning of the Fermi energy level to nearby free surfaces [5]. Changing the band offset at the interface moves the conduction band in one material relative to the valence band in the other, and hence the properties of the system, such as charge transfer between the layers, are very sensitive to the value of the offset.

Figure 1 illustrates the band overlap for a single layer of InAs imbedded in GaSb. It is obvious that, in this case, the band offset is given by the sum of the electron and hole confinement energies and their respective Fermi energies. These various energies can easily be determined. For example, by performing magnetotransport measurements we can find the electron and hole densities and thus their Fermi energies. If, for the given layer thicknesses, we then self-consistently
GaSb

InAS

GaSb

interface layer has been detected by Raman scattering from short-period superlattices grown using the same sequence [7]. Magnetotransport measurements were performed in magnetic fields up to 15 T. These experiments were repeated as a function of hydrostatic pressure for some of the structures. The pressure was applied at room temperature using the liquid medium clamp cell before slowly cooling to 77 K, and then to 4.2 K by immersing the cell in liquid helium.

It is well known that in a single-carrier system the Hall voltage varies linearly with magnetic field. A typical in the InAs/GaSb characteristic system of two-carrier which contains conduction, both electrons such as and holes, is that the Hall resistance traces exhibit an upward curvature with magnetic field. A classical two-carrier fit at low fields is used to extract the electron and hole densities together with their respective mobilities [8].

Fourier transforms of the oscillations in the magnetoresistance traces ($\rho_{xx}$) are used to confirm the fitted densities and also to find the number of occupied subbands. In general the carrier densities for [111]A-oriented structures are more than 50% larger than the equivalent [001] samples, as discussed in reference [9]. The carrier densities for [111]B structures are found to be similar to those for [111]A structures, but the electron mobilities were not sufficient to allow accurate measurement of the Fermi levels.

We find that for [001]-oriented DHETs with wide InAs wells of 600 Å or greater, Fourier transforms of $\rho_{xx}$ traces show that two electron subbands are occupied with equal, or nearly equal, densities [10]. From this we conclude that the two interfaces for [001] growth are identical, and therefore that the confinement potential is symmetrical.

The carrier densities in the structures discussed in this letter are large and cause considerable band bending. The wavefunctions and confinement energies of the electrons and holes together with the associated band bending have been calculated self-consistently, taking into account the energy dependence of the electron mass and the origin of the carriers. Only a brief outline of the calculation is given here, as a more detailed description will be published elsewhere.

Table 1. Carrier densities (per period for the s.l.s) and calculated band overlaps for several [001]-oriented samples. 1132 and 1137 are s.s, all the others are DHETs.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Thicknesses InAs/GaSb (Å)</th>
<th>Electron density (10^{11} cm^{-2})</th>
<th>Hole density (10^{11} cm^{-2})</th>
<th>Band overlap (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>973</td>
<td>300</td>
<td>7.5</td>
<td>4.0</td>
<td>140</td>
</tr>
<tr>
<td>970</td>
<td>450</td>
<td>7.00</td>
<td>3.04</td>
<td>137</td>
</tr>
<tr>
<td>957</td>
<td>600</td>
<td>11.62</td>
<td>0.74</td>
<td>142</td>
</tr>
<tr>
<td>977</td>
<td>1200</td>
<td>10.9</td>
<td>0\textsuperscript{a}</td>
<td>124\textsuperscript{b}</td>
</tr>
<tr>
<td>1249</td>
<td>220/120</td>
<td>6.5</td>
<td>6.2</td>
<td>145</td>
</tr>
<tr>
<td>1132</td>
<td>200/200</td>
<td>7.03</td>
<td>3.14</td>
<td>139</td>
</tr>
<tr>
<td>1137</td>
<td>280/190</td>
<td>7.2</td>
<td>4.8</td>
<td>149</td>
</tr>
</tbody>
</table>

\textsuperscript{a} Not possible to deduce hole density.

\textsuperscript{b} Hole contribution to band overlap not included.
Overall, the structures contain no net charge, and the excess of electron density over hole density is balanced by two regions of fixed positive charge. Firstly, there is a small depletion region in the GaSb due to Fermi energy pinning at the bulk acceptor level of 34 meV above the valence band edge [11]. Secondly, some positive charge is located at each of the interfaces with equal concentrations.

Table 1 shows the calculated band overlap for several [001]-oriented samples. The estimated overlap is within a few meV of 140 meV for all the samples, covering a wide range of structures, which is in very good agreement with the previously measured value of 150 meV [3]. For thin InAs wells the electron wavefunction is very similar to that of an infinite square well, and only one subband is occupied as shown in figure 1. For the relaxed sample with an InAs thickness of 1200 Å, which is in effect two separate heterojunctions, it was not possible to extract a hole density from the transport measurements. Fourier transforms show that the electrons occupy three subbands, two of which have equal concentrations. The electronic contribution to the band overlap has been calculated for this sample and is shown in table 1. We would expect the holes to add a further 10 to 15 meV to the band overlap, thus making the calculated band crossing for even this relaxed sample consistent with those of the other [001] samples.

The band overlaps have been calculated in a similar way for the [111]A samples except that these structures are no longer symmetrical, due to the presence of a strain-induced piezoelectric field. The InAs/GaSb system has a 0.62% lattice mismatch, and the existence of off-axis strain components for [111] growth (which are zero for [001]) induces an electric polarization [12]. The strain-induced piezoelectric fields are 1.9 × 10⁴ V cm⁻¹ and -4.7 × 10⁵ V cm⁻¹ in the InAs and GaSb layers, respectively, for a superlattice with layers of equal thickness. This field has been shown previously to modify both the electrical and optical properties of structures made from a variety of materials [13]. The conduction band of InAs is therefore higher at one interface than at the other, and this asymmetry is balanced by an uneven distribution of the holes between the two interfaces. For DHETs it is assumed that the InAs layer is grown lattice-matched to GaSb. However, for superlattices the strain is symmetrized following the method of Smith [12], and a long-range electric field is added so that the band edges are periodic. Figure 1 shows band energy diagrams, together with the electron wavefunctions and associated confinement energies, for both an [001] and a [111]A DHET. For thin InAs layers the wavefunction has only a single peak, as for [001] structures, but this is displaced from the centre of the well by the piezoelectric field as shown in figure 1.

Table 2 shows the calculated band overlap for several [111]A samples. The band crossing again remains almost constant over a large range of thicknesses and structures but gives a value that is typically 60 to 70 meV larger than for the [001] orientation. There is therefore strong evidence for an orientation dependence of the band overlap.

The existence of this orientation dependence of the band overlap will have significant consequences for a number of properties of this system. For example, we may expect increased interband tunnelling currents due to the larger densities of states, and enhanced peak to valley ratios in negative differential resistance measurements [14]. Recent reports of enhanced interband optical absorption in [111] short-period structures are likely to be related to this orientation dependence of the band overlap [15].

We attribute this orientation dependence of the band overlaps to the presence of a large interface dipole for the [111]A-oriented structures. The origin and magnitude of the dipole contribution to band offsets have been studied for the case of thin surface layers of Ge on GaAs, with theoretical estimates of the order of 1 eV and measured values of the order of 100 meV [2, 16]. In the present case of a single monolayer of InSb at the interface, a transfer of 1% of an electron charge between each pair of InSb atoms is needed to produce a dipole contribution to the band overlap of 50 meV. Alternatively, using the bulk piezoelectric and elastic tensor coefficients, we deduce that the strain in the InSb monolayer is of the order of 6%, giving a dipole potential of the order of 15 meV across the interface. Although this analysis does not account for the whole of the interface dipole, it illustrates the importance of the highly strained binary InSb interface layer, which can only be present in structures where both the cation and anion change across an interface.

It is likely that the interface dipole effects are significantly smaller in the [001]-oriented structures, where Foulon and Priester [17] have predicted that for a GaSb/InAs interface the band overlap is about 20 meV larger if the interface bond is Ga–As than if it is In–Sb. The orientation dependence of the offsets is likely to be much smaller in structures such as GaAs/GaAlAs.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Thickness InAs/GaSb (Å)</th>
<th>Electron density (10¹⁷ cm⁻²)</th>
<th>Hole density (10¹⁷ cm⁻²)</th>
<th>Band overlap (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>963</td>
<td>475</td>
<td>11.5</td>
<td>5.4</td>
<td>201</td>
</tr>
<tr>
<td>957</td>
<td>600</td>
<td>15.02</td>
<td>7.21</td>
<td>192</td>
</tr>
<tr>
<td>977</td>
<td>1200</td>
<td>18.3</td>
<td>2.3</td>
<td>200</td>
</tr>
<tr>
<td>1135</td>
<td>200/200</td>
<td>14.5</td>
<td>6.7</td>
<td>200</td>
</tr>
</tbody>
</table>

Table 2. Carrier densities (per period for the s.u.s) and calculated band overlaps for several [111]A-oriented samples. 1135 is the only s.
The orientation dependence of the overlap is not influenced by the macroscopic strain state of the structures, as evidenced by the fact that the overlaps deduced for the thicker structures with relaxed layers are identical to those for the fully strained structures. In the case of the widest layer [111]A sample with a 1200 Å InAs well, the Fourier transforms of the oscillations show that two of the three occupied electron subbands contain almost the same number of carriers, suggesting a symmetric potential profile. This is strong evidence that the majority of the strain has been relaxed by the formation of misfit dislocations, thus destroying the microscopic piezoelectric field, but still giving the enhanced band overlap.

We have also used hydrostatic pressure to modify the band overlap for both orientations. The bulk moduli of GaSb and InAs are 578 and 580 kbar respectively, so the application of pressure will not induce any additional piezoelectric field in [111]-oriented structures, if it is truly hydrostatic. As the pressure is increased, the bandgaps of GaSb and InAs both increase and the band overlap at the interface decreases, as a result of which electrons transfer from the InAs conduction band back into the valence band of GaSb. Figure 2 shows the experimental magnetotransport traces at various pressures for an [001]-oriented DHET. Both the Hall and magnetoresistance traces are seen to change from those characteristic of two carrier types [18] to the familiar traces expected from a one-carrier system. At low pressure values where the structures contain both electrons and holes, i.e. in the semimetallic regime, \( \rho_{xy} \) is characterized by the strong parabolic dependence on magnetic fields [19] and oscillatory features, and \( \rho_{xx} \) shows very weak oscillations superimposed on a large magnetoresistance background. Once the pressure value is so high that the hole density falls to zero, the magnetoresistance background decreases, and \( \rho_{xx} \) exhibits strong minima, approaching zero, whilst \( \rho_{xy} \) varies linearly with magnetic field along with quantized plateaux [20].

The band overlap has been calculated self-consistently at each pressure for both orientations as described above, and the resulting dependence of band overlap on pressure is shown in figure 3. The change in band overlap with pressure is also found to be slightly orientation dependent, decreasing at rates of 9.9 ± 1.0 and 11.9 ± 1.5 meV kbar\(^{-1}\) for the [001] and [111]A orientations respectively. The difference in the pressure coefficients for the two orientations suggests that the magnitude of the interface dipole is also pressure dependent, as might be expected since the strength of the In-Sb bond is substantially less than In-As or Ga-Sb, as can be seen from the lower bulk modulus of InSb (457 kbar). The rates are substantially larger than those previously determined using MBE samples [20, 21], but much closer to the bandgap variations of bulk GaSb (14 meV kbar\(^{-1}\)) and InAs (10 meV kbar\(^{-1}\)). The model-solid theory of Van de Walle and Martin [1] predicts that the band crossing should decrease with pressure at 10.1 meV kbar\(^{-1}\) for the [001] orientation, which is in very good agreement with our experimental results. We believe that our results are more accurate than those previously measured because of the much lower extrinsic contribution to the doping levels in our MOVPE samples.

In conclusion, we have shown that the band overlap at the GaSb/InAs interface is about 60 meV larger for the [111]A orientation than for the [001], which we attribute

Figure 2. Hall resistance traces (top) and magnetoresistance traces (bottom) for an [001]-oriented DHET with a 300 Å InAs well. The numbers give the pressure in kbar.

Figure 3. Calculated band overlaps for the two DHETs as functions of pressure. The circles show the [001] overlap. Full triangles show the calculated [111]A band overlap up to 9 kbar, but above this the hole density is zero and the open triangles give calculated upper limits from the electron levels alone.
to an interface dipole for [111]A growth. This overlap is also found to decrease at a slightly faster rate with hydrostatic pressure for the [111]A orientation.

References

[18] Nicholas R J 1993 Physica B 184 268