02 Basics of Heterostructures

The limitations of homogeneous semiconductors and homo-junctions

The carrier transport cannot be controlled independently
02 Basics of Heterostructures

The limitations of homogeneous semiconductors and homo-junctions

The potential barriers in the p-n junctions for electrons and holes cannot be controlled independently
The electron and hole confinement (the spatial distribution) cannot be controlled independently.
02 Basics of Heterostructures

**Abrupt Composition**

*Abrupt composition: Forms energy wells and superlattices*
Heterojunctions

The *conventional p-n diode* uses doping profiles to control current. Using *variation in material composition* gives additional degrees of freedom.

Graded composition: May give a different built-in electric field for electrons and holes.
Composite semiconductor structures consisting of two or more layers of different materials, one grown on another, are commonly referred as heterostructures.

Heterostructures for quantum devices are required to have sharp junctions, since for quantization the dimensions are required to be comparable to the electron wavelength, which is of the order of a few nanometers.

Heterostructures are normally grown by either MOCVD or MBE epitaxial techniques
Molecular Beam Epitaxy
Molecular beam epitaxy is a kind of ultrahigh vacuum evaporation in which the atoms or molecules containing the desired atoms are directed from effusion cells to a heated substrate.

The atoms on arriving at the substrate combine on the lattice sites. The flux of the incident beams are determined by the temperature of the effusion cells. The composition of the grown layer may be controlled by opening and closing the shutters in front of the effusion cells, which are kept at predetermined temperatures.
• The shutters in front of the cells may be opened or shut to start or stop a beam within 0.1-0.3 s. The substrate is heated by resistive heaters or by radiation, to a temperature of 400 -700 °C.

• All the effusion cells are kept inside a shroud, cooled with liquid nitrogen. The gases effusing from the cells are collimated by holes in the shroud.

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• The pressure in the chamber is initially in the 10^-9-10^-11 torr range, which is achieved by long-time baking (8 hrs or more at a temperature around 180 °C). This high vacuum is required for ensuring low pressure of ambient impurities.
Lattice Matching and Bandgap Engineering

There are a few binaries, which have nearly equal lattice constant but different band gap, e.g., GaP and Alp; Ge. GaAs, ZnSe and AlAs; InAs, ZnTe, GaSb and AlSb; aSn, InSb and CdTe.

Heterostructures with good crystalline interfaces have been gown using some of these binaries. Examples are: GaAs/AlAs, InAs/GaSb, InAs/AlSb, InSb/CdTe.

For example, \( \text{Al}_x\text{Ga}_{1-x}\text{As} \) has nearly the same lattice constant as GaAs and AlAs;

The direct band gap may, however, be varied between 2.79 eV and 1.51 eV by changing \( x \).
For example, $\text{Al}_x\text{Ga}_{1-x}\text{As}$ has nearly the same lattice constant as GaAs and AlAs; The direct band gap may, however, be varied between 2.79 eV and 1.51 eV by changing $x$. 
Binaries with different lattice constants may also be combined to obtain a ternary with a lattice constant which is equal to that of a third binary.

Ga$_{0.47}$In$_{0.53}$As and Al$_{0.48}$In$_{0.52}$As are examples of ternaries which are lattice-matched to InP. 

*The band gap of the ternary cannot be chosen in this case.*
The lattice constant and the band gap may, however, be chosen independently by combining four elements to realize quaternaries. \( \text{Ga}_x\text{In}_{1-x}\text{As}_y\text{P}_{1-y} \) is an important example of such a quaternary which has the same lattice constant as InP and a band gap which may be adjusted between 0.73 eV and 1.35 eV when \( x \) and \( y \) are chosen according to the following relation: 

\[
x = 0.1894 \frac{y}{(0.4184 - 0.013 y)}
\]
Types of Heterostructures

The potential profile near the heterojunction has step-discontinuities

Heterostructures are named as Type I, Type II and Type III according to the alignment of the bands producing the discontinuity.

In Type I heterostructures, the band gap of one material entirely overlaps that of the other and the potential discontinuities for the conduction band, $\Delta E_c$, and for the valence band, $\Delta E_v$, may be expressed as,

$\Delta E_c = E_{c1} - E_{c2} = f(E_{g1} - E_{g2}) = f\Delta E_g,$

$\Delta E_v = E_{v1} - E_{v2} = (1-f)(E_{g1} - E_{g2}) = (1-f)\Delta E_g,$
Types of Heterostructures

In Type II heterostructures, $E_{v1} > E_{v2}$ and $\Delta E_c$ may or may not be larger than $E_{g1}$. Also, $E_{g2}$ is not necessarily smaller than $E_{g1}$. Heterostructures of Type II, with $\Delta E_c < E_{g1}$ have been named Type II-staggered. Both the conduction-band edge and the valence-band edge of one material being lower than the corresponding band edges of the other material, electrons are confined in one material, while holes are confined in the other material. This type of band alignment occurs, for example, in InAs/Al$_{0.4}$Ga$_{0.6}$Sb heterostructures.
Types of Heterostructures

Type II heterostructures, with $\Delta E_c > E_g1$ have been named Type II-misaligned. In these heterostructures also, electrons and holes are confined separately in the two materials. But, as the valence band of the material, in which the holes are confined, overlaps the conduction band of the other material some novel phenomena result. InAs/GaSb heterostructure belongs to this class.
Types of Heterostructures

Type III heterostructures are formed by the combination of a semimetal with inverted bands and a semiconductor. HgTe/CdTe is an example of this type of heterostructure.

It should be mentioned that there is some confusion in the literature about the nomenclature of Type III; Type II-misaligned has been named Type III by some authors.
Band Offsets in the Heterostructures

The potential discontinuity (or the so-called band offset) plays a crucial role in quantum devices as it is this discontinuity which causes the quantum behavior of the structures.

Empirical Rules

ELECTRON AFFINITY RULE
The oldest rule is that given by Anderson. According to this rule, the discontinuity in the conduction band edges is the difference of the electron affinities for the constituents, i.e., the conduction band offset,

\[ \Delta E_c = x_1 - x_2, \]

where \( x_1 \) and \( x_2 \) are the electron affinities of material 1 and 2 constituting the heterojunction.

COMMON ANION RULE
This rule is based on the empirical results obtained from the Schottky contacts to III-V and II-VI compounds. The Schottky barrier for the valence band of these compounds to gold has been found to be the same for different compounds containing the same anion.
Experimental Methods

ABSORPTION MEASUREMENT

Quantum wells are realized by sandwiching a thin layer of the lower-band-gap constituent, between two layers of the larger-band-gap material. The absorption spectrum of such structures show peaks corresponding to transitions from the hole levels to the electron levels at near-liquid-helium temperature. Band offsets are determined by fitting the transition energies with the calculated values for different offsets. The method is not very accurate.
Experimental Methods

PHOTOLUMINESCENCE MEASUREMENT
Strong light from a laser is shone on the sample to excite electrons from the valence band to the conduction band. These excited electrons finally recombine to produce the luminescence radiation, giving effectively the shift in band gap due to quantization. Such luminescence lines are recorded for different well widths. The band offset is then obtained by fitting the calculated energy shifts with the measured values.

Theoretical Methods: give values agreeing with the experiments to within 0.1 eV
Values of Band Offset

Accurate values of band offset are difficult to determine.

Attempts for determining its value often yielded widely varying values of band offset.

For example, initially the ratio $\Delta E_c/\Delta E_v$ for the GaAs/Ga$_{0.7}$Al$_{0.3}$As system was fixed to be 85:15, but later experiments established a value of 60:40.

The value of $\Delta E_c/\Delta E_v$ for Ga$_{0.47}$In$_{0.53}$As/InP is reported to be between 36:64 and 100:0.

For the GaInP/GaAs system the offsets vary between 8:92 and 90:10.
Valence-Band offset, $\Delta E_v$, in heterojunctions

<table>
<thead>
<tr>
<th>Heterojunction material</th>
<th>$\Delta E_v$(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaAs/$\text{Al}<em>{x}\text{Ga}</em>{1-x}\text{As}$</td>
<td>0.46x</td>
</tr>
<tr>
<td>GaAs/AlAs</td>
<td>0.31</td>
</tr>
<tr>
<td>GaAs/InAs</td>
<td>0.35</td>
</tr>
<tr>
<td>AlAs/Al$<em>{0.37}$Ga$</em>{0.63}$As</td>
<td>0.34</td>
</tr>
<tr>
<td>AlAs/InAs</td>
<td>0.35</td>
</tr>
<tr>
<td>InP/Ga$<em>{0.47}$In$</em>{0.53}$As</td>
<td>0.32</td>
</tr>
<tr>
<td>GaAS/ALSb</td>
<td>0.40</td>
</tr>
<tr>
<td>GaSb/InAs$<em>{0.95}$Sb$</em>{0.05}$</td>
<td>0.67</td>
</tr>
<tr>
<td>CdTe/HgTe</td>
<td>0.34</td>
</tr>
<tr>
<td>CdTe/ ZnTe</td>
<td>0.40</td>
</tr>
<tr>
<td>ZnTe/HgTe</td>
<td>0.30</td>
</tr>
<tr>
<td>GaN/AlN</td>
<td>0.7±.24</td>
</tr>
<tr>
<td>AlN/GaN</td>
<td>0.57±0.22</td>
</tr>
<tr>
<td>InN/AlN</td>
<td>1.81±0.2</td>
</tr>
<tr>
<td>InN/GaN</td>
<td>1.051</td>
</tr>
<tr>
<td>Al$<em>{0.48}$In$</em>{0.52}$As/Ga$<em>{0.47}$In$</em>{0.47}$As</td>
<td>0.75</td>
</tr>
<tr>
<td>GaSb/InAs</td>
<td>0.51</td>
</tr>
<tr>
<td>AlN/InN</td>
<td>1.32±0.14</td>
</tr>
<tr>
<td>Ga$<em>{0.5}$In$</em>{0.5}$P/GaAs</td>
<td>0.32</td>
</tr>
</tbody>
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