2. Heterojunction material systems

In this section we will discuss three types of material systems: materials made of group IV elements and compound materials made from group III and group V or group II and group VI elements. The more common materials are shown in the figure indicating the energy bandgap as a function of the lattice constant. Since lattice matching is desirable for good quality heterojunctions, one frequently finds that primarily materials on the same vertical line are combined with each other. However lattice mis-matching is also used on purpose to obtain materials with new and interesting properties due to the tensile or compressive strain caused by the mismatch in lattice constant. The figure below also displays alloys of different semiconductors which typically have a lattice constant which varies depending on the composition of the alloy. Ternary alloys form a line on the figure whereas quaternary alloys cover the area between the elemental or compound semiconductors.
Fig. 2.1  Energy bandgap versus lattice constant of some commonly used group IV, III-V and II-VI materials.

Numeric data for different commonly used semiconductors are listed in the table below:
<table>
<thead>
<tr>
<th>Class</th>
<th>Material</th>
<th>Lattice Constant [Å]</th>
<th>Bandgap [eV]</th>
<th>Absorption edge [µm]</th>
<th>Crystal structure</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>IV</td>
<td>Diamond</td>
<td>3.56683</td>
<td>5.47</td>
<td>0.226508</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td>IV</td>
<td>Si</td>
<td>5.43095</td>
<td>1.12</td>
<td>1.10625</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td>IV</td>
<td>Ge</td>
<td>5.64613</td>
<td>0.66</td>
<td>1.877273</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td>IV</td>
<td>Sn</td>
<td>6.4892</td>
<td>0.082</td>
<td>15.10976</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td>IV-IV</td>
<td>6H-SiC</td>
<td>3.086</td>
<td>2.996</td>
<td>0.41355</td>
<td>W</td>
<td>c = 15.117</td>
</tr>
<tr>
<td>III-V</td>
<td>GaAs</td>
<td>5.6533</td>
<td>1.424</td>
<td>0.870084</td>
<td>Z</td>
<td></td>
</tr>
<tr>
<td>III-V</td>
<td>AlAs</td>
<td>5.6605</td>
<td>2.17</td>
<td>0.571494</td>
<td>Z</td>
<td></td>
</tr>
<tr>
<td>III-V</td>
<td>InAs</td>
<td>6.0584</td>
<td>0.36</td>
<td>3.441667</td>
<td>Z</td>
<td></td>
</tr>
<tr>
<td>III-V</td>
<td>InP</td>
<td>5.8686</td>
<td>1.35</td>
<td>0.917778</td>
<td>Z</td>
<td></td>
</tr>
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<td>III-V</td>
<td>GaP</td>
<td>5.4512</td>
<td>2.26</td>
<td>0.54823</td>
<td>Z</td>
<td></td>
</tr>
<tr>
<td>III-V</td>
<td>AlSb</td>
<td>6.1355</td>
<td>1.58</td>
<td>0.784177</td>
<td>Z</td>
<td></td>
</tr>
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<td>III-V</td>
<td>GaSb</td>
<td>6.0959</td>
<td>0.72</td>
<td>1.720833</td>
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<td></td>
</tr>
<tr>
<td>III-V</td>
<td>AlP</td>
<td>5.451</td>
<td>2.5</td>
<td>0.4956</td>
<td>Z</td>
<td></td>
</tr>
<tr>
<td>III-V</td>
<td>InSb</td>
<td>6.4794</td>
<td>0.2</td>
<td>6.195</td>
<td>Z</td>
<td></td>
</tr>
<tr>
<td>III-V</td>
<td>GaN</td>
<td>3.189</td>
<td>3.36</td>
<td>0.36875</td>
<td>W</td>
<td>c = 5.185</td>
</tr>
<tr>
<td>II-VI</td>
<td>ZnS</td>
<td>5.42</td>
<td>3.68</td>
<td>0.336685</td>
<td>Z</td>
<td></td>
</tr>
<tr>
<td>II-VI</td>
<td>CdS</td>
<td>5.832</td>
<td>2.42</td>
<td>0.511983</td>
<td>Z</td>
<td></td>
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<tr>
<td>II-VI</td>
<td>ZnSe</td>
<td>5.65</td>
<td>2.7</td>
<td>0.458889</td>
<td>Z</td>
<td></td>
</tr>
<tr>
<td>II-VI</td>
<td>CdSe</td>
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<td>1.7</td>
<td>0.728824</td>
<td>Z</td>
<td></td>
</tr>
<tr>
<td>II-VI</td>
<td>CdTe</td>
<td>6.48</td>
<td>1.55</td>
<td>0.799355</td>
<td>Z</td>
<td></td>
</tr>
<tr>
<td>ternary</td>
<td>In_{0.53}Ga_{0.47}As</td>
<td>5.8686</td>
<td>0.74</td>
<td>1.671253</td>
<td>Z</td>
<td>Lattice matched to InP</td>
</tr>
<tr>
<td>ternary</td>
<td>Al_{0.48}In_{0.52}As</td>
<td>5.8686</td>
<td>1.46</td>
<td>0.8486</td>
<td>Z</td>
<td>Lattice matched to InP</td>
</tr>
<tr>
<td>ternary</td>
<td>In_{0.5}Ga_{0.5}P</td>
<td>5.6533</td>
<td>1.80</td>
<td>0.688</td>
<td>Z</td>
<td>Lattice matched to GaAs</td>
</tr>
<tr>
<td>ternary</td>
<td>In_{0.5}Al_{0.5}P</td>
<td>5.6533</td>
<td>2.35</td>
<td>0.527234</td>
<td>Z</td>
<td>Lattice matched to GaAs</td>
</tr>
</tbody>
</table>

Table 1. Lattice constants, bandgap energy and absorption edge of different semiconductors and alloys.

\[D = \text{Diamond lattice, } Z = \text{Zincblende lattice, } W = \text{Wurtzite lattice}\]
2.1 The GaAs/AlGaAs material system

The GaAs/AlGaAs material system is one of the commonly used material systems. Its main advantage is that the material is closely lattice matched\(^2\) for any aluminum fraction. The energy of the conduction and valence band edges are shown in the figure below.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{band_edges.png}
\caption{Valence band edge \(E_v\), conduction band edge for the \(\Gamma\) minimum, \(E_{c\Gamma}\), the L minimum, \(E_{cL}\) and the X minimum \(E_{cX}\) as a function of the aluminum fraction.}
\end{figure}

\(\text{2The actual mismatch between GaAs and AlAs is only 0.127\%.}\)
The figure contains three conduction bands corresponding to two different band minima, namely the \( \Gamma \), L and the X minimum. The figure can be used to extract the conduction and valence band discontinuities between two \( \text{Al}_x\text{Ga}_{1-x}\text{As} \) materials with different aluminum fraction \( x \). It can also be used to obtain the minimum band gap of the material. Since the \( \Gamma \) minimum forms a direct bandgap and the X minimum an indirect bandgap, one finds that the \( \text{Al}_x\text{Ga}_{1-x}\text{As} \) becomes indirect for \( x > 0.45 \). The L minimum does not affect the minimal energy bandgap for any aluminum fraction\(^3\). The numeric values corresponding to Fig. 2.2 are shown in Table 2.

\(^3\)The L minimum does play a role in carrier transport under high field conditions, causing the Gunn effect in GaAs.
Table 2. Conduction and valence band energies of Al$_x$Ga$_{1-x}$As versus aluminum fraction

The numeric values were calculated from the following expressions:

$\Delta E_{g1} = 1.247 \times x$

$\Delta E_{g2} = 0.476 + 0.125 \times x + 0.143 \times x^2$

$\Delta E_c = \Delta E_g - \Delta E_v$

$E_v = -0.4 \Delta E_{g1}$

$E_g \Gamma = 1.424 + \Delta E_{g1}$

$E_g X = 1.424 + \Delta E_{g2}$

$E_c \Gamma = 1.424 + 0.6 \Delta E_{g1}$

$E_c X = 1.424 - 0.4 \Delta E_{g1}$

$E_{cL} \equiv 1.73 + 0.4 \times x$
A more extensive list\textsuperscript{4} of material parameters can be found in Table 3.

<table>
<thead>
<tr>
<th>$x$</th>
<th>$\varepsilon_r$</th>
<th>$m_n^*$</th>
<th>$m_p^*$</th>
<th>$E_g$ [eV]</th>
<th>$N_c$ [cm$^{-3}$]</th>
<th>$N_v$ [cm$^{-3}$]</th>
<th>$n_i$ [cm$^{-3}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>13.80</td>
<td>0.067</td>
<td>0.62</td>
<td>1.42</td>
<td>4.343E+17</td>
<td>1.223E+19</td>
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<tr>
<td>0.05</td>
<td>13.64</td>
<td>0.07115</td>
<td>0.627</td>
<td>1.49</td>
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<tr>
<td>0.10</td>
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<td>0.0753</td>
<td>0.634</td>
<td>1.55</td>
<td>5.175E+17</td>
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<tr>
<td>0.15</td>
<td>13.33</td>
<td>0.07945</td>
<td>0.641</td>
<td>1.61</td>
<td>5.608E+17</td>
<td>1.285E+19</td>
<td>77948.1</td>
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<tr>
<td>0.20</td>
<td>13.18</td>
<td>0.0836</td>
<td>0.648</td>
<td>1.67</td>
<td>6.053E+17</td>
<td>1.306E+19</td>
<td>24435.6</td>
</tr>
<tr>
<td>0.25</td>
<td>13.02</td>
<td>0.08775</td>
<td>0.655</td>
<td>1.74</td>
<td>6.51E+17</td>
<td>1.328E+19</td>
<td>7645.35</td>
</tr>
<tr>
<td>0.30</td>
<td>12.86</td>
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<td>0.662</td>
<td>1.80</td>
<td>6.977E+17</td>
<td>1.349E+19</td>
<td>2387.84</td>
</tr>
<tr>
<td>0.35</td>
<td>12.71</td>
<td>0.09605</td>
<td>0.669</td>
<td>1.86</td>
<td>7.455E+17</td>
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<tr>
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<tr>
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<tr>
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<td>0.69</td>
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<td>1.725E+19</td>
<td>1.435E+19</td>
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</tr>
<tr>
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<tr>
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<td>1.656E+19</td>
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</tr>
<tr>
<td>0.70</td>
<td>11.62</td>
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<td>2.06</td>
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</tr>
<tr>
<td>0.75</td>
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<td>0.725</td>
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<td>1.61E+19</td>
<td>1.546E+19</td>
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</tr>
<tr>
<td>0.80</td>
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<td>0.732</td>
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<td>1.588E+19</td>
<td>1.568E+19</td>
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</tr>
<tr>
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<td>0.739</td>
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<td>1.591E+19</td>
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<tr>
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<td>0.746</td>
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</tr>
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<td>0.76</td>
<td>2.17</td>
<td>1.498E+19</td>
<td>1.659E+19</td>
<td>9.56726</td>
</tr>
</tbody>
</table>

Table 3. Material parameters for Al$_x$Ga$_{1-x}$As

The existence of several conduction band minima as well as several conduction band maxima leads to the question of what the correct effective density of states is for the whole band. This question can simply be answered by stating that the total carrier density equals the sum of the densities in each of the minima/maxima, or:

\[ n = n_{\Gamma} + n_{L} + n_{X} \]

\[ = N_{c\Gamma} \exp[(E_{fn} - E_{c\Gamma})/kT] + N_{cL} \exp[(E_{fn} - E_{cL})/kT] + N_{cX} \exp[(E_{fn} - E_{cX})/kT] \]

which assuming \( E_{c\Gamma} \) to be smallest of the three conduction band edges, can be rewritten as:

\[ n = N_{c\Gamma}^{\ast} \exp[(E_{fn} - E_{c\Gamma})/kT] \]

with

\[ N_{c\Gamma}^{\ast} = N_{c\Gamma} + N_{cL} \exp[(E_{c\Gamma} - E_{cL})/kT] + N_{cX} \exp[(E_{c\Gamma} - E_{cX})/kT] \]

The values in the table are calculated using this procedure. In addition it should be noted that the resulting value for the effective density of states can only be used for non-degenerate semiconductors.
2.2 Strained GaInAs material

Ternary GaInAs can be grown on GaAs in spite of the lattice mismatch as long as one does not exceed the critical thickness. This material is used in the base of high-speed hetero-junction bipolar transistors, as a quantum well material for long-wavelength lasers and detectors and as contact layers for non-alloyed contacts. The strain removes the valence band degeneracy so that light holes are energetically favored over the heavy holes. The separation of the maximum of the light hole and heavy hole band equals 4.7meV per percent indium.

![Graph showing energy band gap, absorption edge, and lattice mismatch versus In fraction.](image)

Fig. 2.3 Energy band gap, absorption edge and lattice mismatch versus Indium concentration of strained Ga$_{1-x}$In$_x$As.