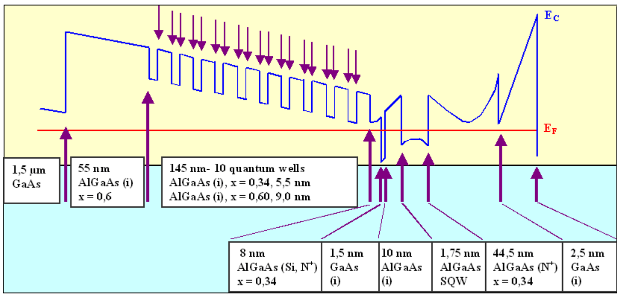
5.3 Heterojunctions

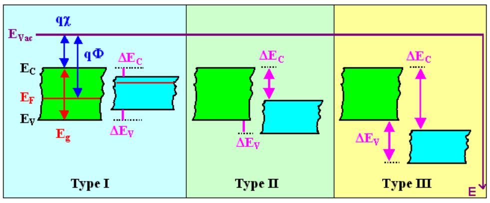
5.3.1 Ideal Heterojunctions

General Remarks

- Optoelectronics, as well as practically all other devices made of compound semiconductors, always contain **heterojunctions**, i.e., junctions between two different semiconductors, for a variety of reasons.
  - One possible reason was already mentioned: Transparency to light generated in some active part.
  - But there are many other advantages so compelling that extremely complicated heterostructures are now routinely produced despite a lot of problems that are encountered, too.
  - Below, the conduction band structure of an advanced **$Al_xGa_{1-x}As$** device is shown to illustrate that point. The doping is shown in brackets; "**i**" means undoped (= intrinsic). **SQW** is short for "Single Quantum Well" – whatever that may be.
  - There are many different heterojunctions, so we will not be able to delve very deep into the subject. The logic behind this structure will be made clear in a later chapter.



- In this sub-chapter we will look at some major properties of heterojunctions. First of all: *How do we construct a band diagram*?
  - Let's first look at the basic cases that we may encounter when considering heterojunctions. Naturally, the bandgaps are always different, but only specifying E_g**(1)** and E_g**(2)** [and of course the Fermi energy in **(1)** and **(2)**] is *not* sufficient to describe the heterosystem before the contact of the materials **(1)** and **(2)**.
  - *We also must specify the exact position on the energy scale of one of the band edges*. This then gives rise to *three* distinct cases for heterojunctions as illustrated below together with the necessary definitions of the various energies needed.
  - You may want to consult a special module (*in German*) dealing with some of the questions that may come up.

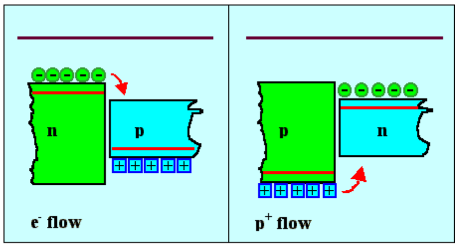


- Looking at the left hand case (Type **I**), we first discuss the various energies encountered:
  - In contrast to "simple" band diagrams in **Si**, the vacuum energy level is now included (and defines the zero point of the energy axis). We also have the energy of the band edges, E_C and E_V, and from their difference the bandgap energy E_g.
  - By convention, the difference between the conduction band edge and the vacuum energy is defined as a potential called "**electron affinity** χ"; $q \cdot \chi$ is thus the work needed to move a charge from the (lower) conduction band edge to infinity.
  - *Note that this is not exactly the same as the electron affinity in more chemical oriented lingo, where it is the energy gained by the reaction $X + e^- = X^-$ and thus only defined by atoms that form stable negatively charged ions*.
  - The difference between the Fermi energy and the vacuum energy is given by charge times the **workfunction** Θ of the material, **q** · Θ is thus the energy needed to move a *fictitious* electron (because in semiconductors usually there is none at the Fermi energy) from the Fermi energy to infinity.
  - *Note that while χ is a material constant, Θ is not – it changes with the position of the Fermi energy.*
  - We may also define the differences of the band edges between the two materials, ΔE_C and ΔE_V, although they are implicitly given by the prime material parameters χ and $E_g = E_C - E_V$.

- The three types of heterojunctions possible are:
    - **Type I (straddling):** The bandgap of one semiconductor is completely contained in the bandgap of the other one; i.e. $E_C(2) > E_V(1)$ and $E_V(2) < E_V(1)$. The discontinuities of the bands are such that both types of carriers, electrons and holes, need energy (ΔE_C and ΔE_V, resp.) to change from the material with the smaller band gap to the one with the larger gap – the carriers from the other side loose this energy when they cross the junction. Type **I** heterojunctions are quite common, the important **GaAs/AlGaAs** system belongs to this kind.
    - **Type II (staggered):** The bandgaps overlap, but one $\Delta E_{C \text{ or } V}$ changes sign. The situation with respect to moving carriers from **(1)** to **(2)** or vice verse is no longer symmetrical. One kind of carrier gains energy (in the example if electrons move from right to left), the other one needs energy (the holes). The **InP/InSb** system provides an example.
    - **Type III (broken-gap):** The bandgaps do not overlap at all. The situation for carrier transfer is like type **II**, just more pronounced. The system **GaSb/InAs** belongs to this type.

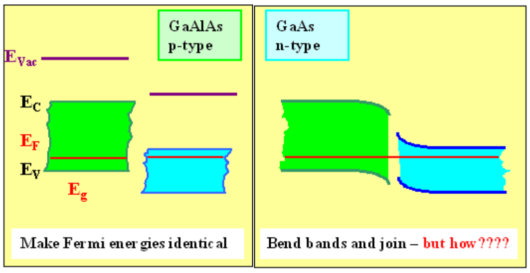
Construction of Band Diagrams

- What happens if we join the two materials? Exactly the same thing as for differently doped Si:
    - Carriers will flow across the junction, building space charges (and now possibly also interface charges) until the Fermi energy is the same everywhere in the material. Far away from the junction, everything is unchanged.
    - However, there are pronounced differences to the case of a **p–n** junction in **Si**. Let's imagine symmetrical junctions, i.e. the majority carrier density is identical in the **p-** and **n**-part. For *homojunctions* , the number of electrons flowing into the **p**-type part is then the same as the number of electrons flowing into the **n**-part. However, at least in the type **I** case, only *one kind of carrier will flow* as is obvious and shown below. The space charge regions to the left and right of the junction thus might not be symmetric.



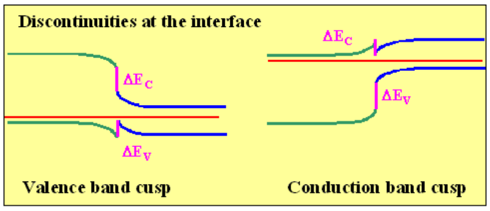
- Still, some kind of carrier transfer will happen and the electrostatic potential far away from the junction will rise from a constant level on one side to a different, but constant level on the other side. The difference will be equal to the difference in Fermi energy before the contact divided by the elementary charge. To the left and the right of the junction the bands are bend accordingly, and so is the vacuum energy.

- Let's see how far this recipe takes us with a simple **GaAs–AlGaAs** type **I** junction:



- First, we align the Fermi energies. Then, we bend the bands – in a smaller region on the more heavily doped side, but always identical for both band edges! After all, the vacuum potential at some position x is fixed and so are the band edges relative to the vacuum potential.

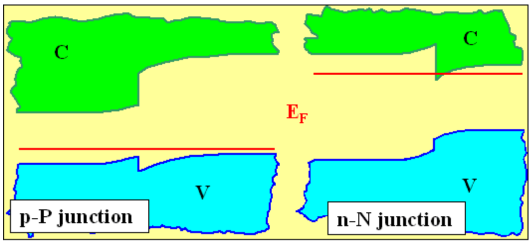
- This leaves us with something new: ***We cannot join the bands of the two materials!*** If we adjust the band bending on both sides so that the conduction bands match, the valence band won't match and vice verse. We must introduce a **discontinuity** right at the interface at one of the bands – or at both.
    - The next picture shows how to do that for type **I** heterojunctions for both possible doping cases.



  - Some kind of cusp or notch must form in the conduction or valence band, depending on the details of the system. Exactly what happens and what the cusps look like depends on many details, you must solve the Poisson equation properly for a specific case.
  - Again, a discontinuity like this *must happen*, even at "ideal" interfaces. We don't know exactly what it looks like, but we can now take this potential and plug it into a one-dimensional Poisson equations and see what it means for the charge distribution.
  - Unavoidably, there must be a *dipole layer* right at the interface (look at this basic module if you have problems figuring that out). The distance between the charges of this dipole layer is so small, however (atomic size) that it does not influence the carrier movement (there is an acceleration/de-acceleration process with equal magnitudes at a very small scale in classical terms or effortless **tunneling** in quantum-mechanical terms).
  - This dipole layer with its sharp wiggle in the charge distribution is therefore usually not included in drawings of the heterojunction.

- In reality, the matching of two lattice types with different atoms on both sides may well introduce some **interface states** in the bandgap, as discussed for the free **Si** surface.
  - Depending on the Fermi energy (which is of course influenced by the interface states, too), these interface states may be charged and introduce some band bending of their own.

- To make things even more complicated (for *pessimists*), or to add more possibilities for engineering with heterojunction (for *optimists*), we now can produce junctions with specific properties between materials of the *same* doping type – even for identical carrier densities.
  - This type of heterojunction is sometimes called an **isotype junction** , the **p–n** type a **diode-type junction**. Some people use abbreviations, with upper case letters indicating the doping type of the material with the wider bandgap and lower case letters the other one. We then have **Pn**, **pN**, **Np**, and **nP** junctions of the *diode* type, and **Nn**, **nN**, **Pp**, and **pP** junctions of the *isotype*. If we look ahead, we can now easily denote multi-junctions like **PnP**, and so on.
  - Also isotype junctions have band discontinuities at the interface, and also here the cusp is where the Fermi energy is; the next picture shows examples.



  - You may already wonder what properties to expect from this kind of junction and what it is good for; we will discuss that later.

- We now have a degree of freedom for all heterojunctions, which did not occur for homojunctions: *How do we distribute the discontinuity?*
  - In the left hand diagrams above, e.g., we could decrease ΔE_C and increase ΔE_V by an identical amount, making the cusp more pronounced; or we do it the other way around. How can we find the real case?
  - The answer is: Nobody knows how to do that in some kind of comprehensive theory. The simplest model (called the **Anderson** model) assumes that ΔE_C is equal to the difference in the electron affinities χ:

$$\Delta E_C = q \cdot [\chi(2) - \chi(1)]$$

  - But that is only a rough estimate that may be quite wrong – not to mention that *bulk* electron affinities cannot be calculated with any precision, and measurements always obtain the (systematically different) *surface* electron affinities.

- There is, however, one feature of the discontinuities that makes life somewhat easier: Whatever its value, it is determined by the interaction of the atoms at the interface and interatomic forces are responsible for its value.
  - This simply means that its value does not change much if we change properties of the materials on a scale much larger than the atomic scale. In other words:

- The band bending necessary for adjusting the potentials on both sides of the junction, so that the Fermi energy is identical, may be seen as independent of the value of the discontinuities. If we construct a band diagram, we simply always keep the same value for the discontinuities (as determined from using the vacuum level as reference for the separate bulk materials), no matter what else we do with the bands.

Properties of Heterojunctions

How do we measure the values of the discontinuities? The answer is: Make the heterojunction and *measure* the junction properties.

- In order to do that, we need to know how the discontinuities influence measurable quantities. How, for example, does the precise nature of the discontinuities influence the current–voltage characteristic of a heterojunction? Or, if there is some radiative recombination, the quantum- or current efficiencies?
- *We are now entering deep water*. Or are we? After all, the equations for ***I–V*** characteristics of a junction (without the space charge layer part) in the simple or more complex form did not contain anything about the shape of the band bending – only the potential difference and bulk properties of materials to the left and right of the junction.
- This tells us that the basic diode characteristics (assuming that nothing happens in the space charge region) must still be valid in its general form, but with *one big difference* that transfers into a decisive property of heterojunctions:
- The hole and electron part of the total current now are *different* even for a perfectly symmetric junction!

This is most easily seen if we look at the relation between the two partial currents j_e and j_h, called the injection ratio $\kappa = j_e / j_h$. Taking the expressions from the simple diode equation given before, we obtain

$$\kappa = \frac{j_e}{j_h} = \frac{e \cdot n_e^{p} \cdot D_e / L_e}{e \cdot n_h^{n} \cdot D_h / L_h}$$

- Rewriting this in terms of the carrier mobilities and the doping densities (assuming fully ionized dopants) with the relations given before, we obtain

$$\kappa = \frac{[\mu_e \cdot n_i{}^2 / (L_e \cdot N_A)]_{\text{p-side}}}{[\mu_h \cdot n_i{}^2 / (L_h \cdot N_D)]_{\text{n-side}}}$$

- For homojunctions, the intrinsic carrier density n_i is the same on both sides, *but not for heterojunctions!* For the intrinsic carrier densities of any semiconductor we have the basic equations:

$$n^e{}_i = N^e{}_{\text{eff}} \cdot \exp\left(-\frac{E_C - E_{Fi}}{kT}\right)$$

$$n^h{}_i = N^h{}_{\text{eff}} \cdot \exp\left(-\frac{E_{Fi} - E_V}{kT}\right) = n^e{}_i$$

- With E_{Fi} = Fermi energy for the intrinsic case.

Only for the case that $N^e{}_{\text{eff}} = N^h{}_{\text{eff}}$ would the Fermi energy be in the middle of the band gap; and while we always used that approximation for **Si**, we must be more careful with compound semiconductors.

- But independent of the exact position of the Fermi energy, for total equilibrium we always have

$$n_i{}^2 = n^e{}_i \cdot n^h{}_i = N^e{}_{\text{eff}} \cdot N^h{}_{\text{eff}} \cdot \exp\left(-\frac{E_C - E_V}{kT}\right)$$

- Inserting this relation into the equation for the injection ratio κ from above, introducing the difference of the band gaps of material **1** and material **2** as $\Delta E_g = E_g(1) - E_g(2)$, and substituting "**1**" and "**2**" for "**n-side**" and "**p-side**" (because this relation is valid for *any* heterojunction of the diode type), we obtain for κ:

$$\kappa \;=\; \frac{[\,\mu_e \cdot N_{\text{eff}}{}^{e} \cdot N_{\text{eff}}{}^{h} \,/\, (L_e \cdot N_A\,)]_1}{[\,\mu_h \cdot N_{\text{eff}}{}^{e} \cdot N_{\text{eff}}{}^{h} \,/\, (L_h \cdot N_D)]_2} \cdot \exp\left(-\,\frac{\Delta E_g}{kT}\right)$$

- This is a very important equation for optoelectronics. Let's see why:
  - If ΔE_g is sufficiently large – and since it is in an exponential term, it does not have to be *very* large – it will always overwhelm the possible asymmetries in the pre-exponential term, e.g. because of different doping levels, or effective density of states between the two materials, and this means $\kappa = j_e / j_h$ is very different from **1**. Getting all signs right, we have the following situation:

Junction type	ΔE_g	**exp** $[-\Delta\, E_g/(kT)]$	κ
Pn	>0	small	small
pN	<0	large	large

  - In other words: *In heterojunctions of the diode type, injection of the majority carriers from the material with the larger band gap (almost) always far surpasses the reverse process*.
  - To give a relevant example: For a **GaAs/Ga$_{0.7}$Al$_{0.3}$ As** junction with ΔE_g **= 0.3 eV** and for doping densities of $\mathbf{10^{18}}$ $\mathbf{cm^{-3}}$ or $\mathbf{2 \cdot 10^{17}}$ $\mathbf{cm^{-3}}$, respectively, we have $\kappa \approx \mathbf{10^6}$**.**
- Why is a large value of κ so important?
  - Because if we sandwich a *small* gap semiconductor between two *large* gap semiconductors, we should be able to inject a lot of electrons from one side and a lot of holes from the other side – with no means of escape. The injected carriers *must* recombine in the small gap part, which thus is our recombination zone – we have a large current efficiency η_{cu}.
  - If you think about that a minute and try to come up with some structure, you will realize that there is a problem: You cannot have injection via *two* **p–n** junctions – one junction must be an isotype junction. But luckily, isotype junctions have similar properties: it is easy to inject majority carriers from the wide band gap side and not so easy from the other side.