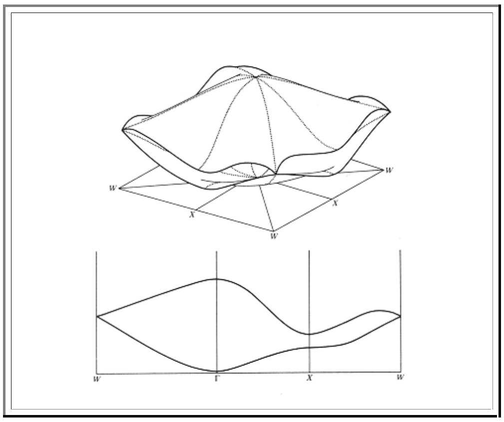
### 2.1.5 Band Structures and Standard Representations

Real crystals are three-dimensional and we must consider their band structure in three dimensions, too.

- Of course, we must consider the reciprocal lattice, and, as always if we look at electronic properties, use the Wigner-Seitz cell (identical to the **1st** Brillouin zone) as the unit cell.
- There is no way to express quantities that change as a function of three coordinates graphically, so we look at a two dimensional crystal first (which, incidentally, do exist in semiconductor physics).

The qualitative recipe for obtaining the band structure of a two-dimensional lattice using the slightly adjusted parabolas of the free electron gas model is simple:

- Construct the parabolas along major directions of the reciprocal lattice, interpolate in between, and fold them back into the first Brillouin zone. How this can be done for the free electron gas is shown in an illustration module.
- An example – taken from "Harrison" – may look like this:



- The lower part (the "cup") is contained in the **1st** Brillouin zone, the upper part (the "top") comes from the second **BZ**, but is now folded back into the first one. It thus would carry a different band index. This could be continued ad infinitum; but Brillouin zones with energies well above the Fermi energy are of no real interest.
- The lower part shows tracings along major directions. Evidently, they contain most of the relevant information in condensed form. It is clear, e.g., that this structure has no band gap.

It would be sufficient for most purposes to know the $\mathbf{E}_n(\boldsymbol{k})$ curves – the dispersion relations – along the major directions of the reciprocal lattice (***n*** is the band index) (see quantum mechanics script as well).

- This is exactly what is done when real band diagrams of crystals are shown. Directions are chosen that lead from the center of the Wigner-Seitz unit cell – or the Brillouin zones in the more generalized picture – to special symmetry points. These points are labeled according to the following rules:
    - Points (and lines) inside the Brillouin zone are denoted with *Greek* letters.
    - Points on the surface of the Brillouin zone with *Roman* letters.
    - The center of the Wigner-Seitz cell is always denoted by a **Γ**
- For cubic reciprocal lattices, the points with a high symmetry on the Wigner-Seitz cell are the intersections of the Wigner Seitz cell with the low-indexed directions in the cubic elementary cell.
- We use the following nomenclature: ( red for **fcc**, blue for **bcc**):

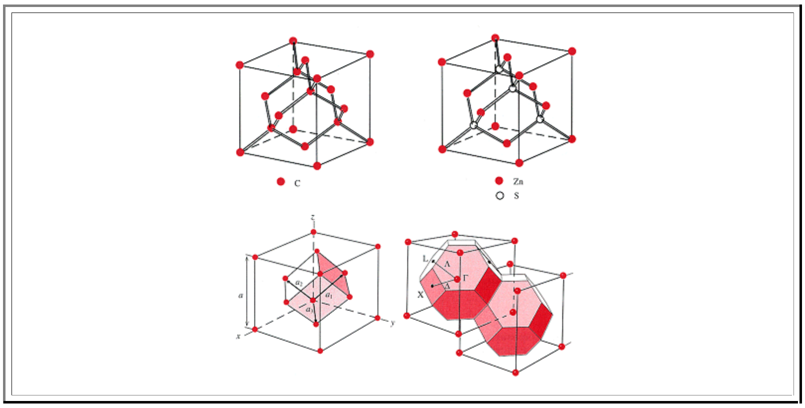
The intersection point with the **[100]** direction is called **X** (**H**); the line **Γ—X** is called Δ.

The intersection point with the **[110]** direction is called **K** (**N**); the line **Γ—K** is called Σ.

The intersection point with the **[111]** direction is called **L** (**P**); the line **Γ—L** is called Λ .

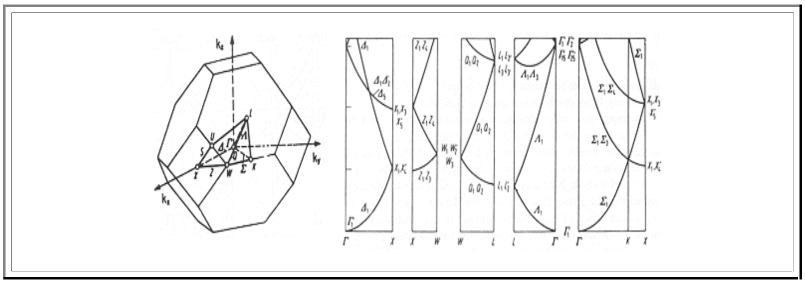
The picture above already used this kind of labelling. Since the tracing of the dispersion curve can be done on different levels – corresponding to the **1st**, second, etc. Brillouin zone – the points are often indexed with the number of the Brillouin zone they use.

- This may look like this:



- The top pictures show the elementary cell of the diamond lattice or of the ZnS type lattice; the lower left picture the Bravais lattice of the **fcc** type and the primitive (non-cubic) lattice which is an equally valid, if less symmetric, representation of the **fcc** lattice..
- The lower right picture shows the cubic reciprocal lattice of the cubic **fcc** lattice (which is a **bcc** lattice) and the Wigner-Seitz cells (identical with the first Brillouin zone) which also represent the reciprocal lattice

We now can draw the band diagrams along all kinds of lines – not only from **Γ** to some point on the Brillouin zone, but also from point to point, e.g., from **L** to **K** or to some other points not yet labeled. An example for the **fcc** structure and the *free electron gas approximation* is shown below.



- The first Brillouin zone with the proper indexing of the relevant points and some dispersion parabola along prominent directions are shown. The picture is taken from Hummel's book.
- The indexing of the various branches is a bit more complicated than in the illustration example for reasons explained below.

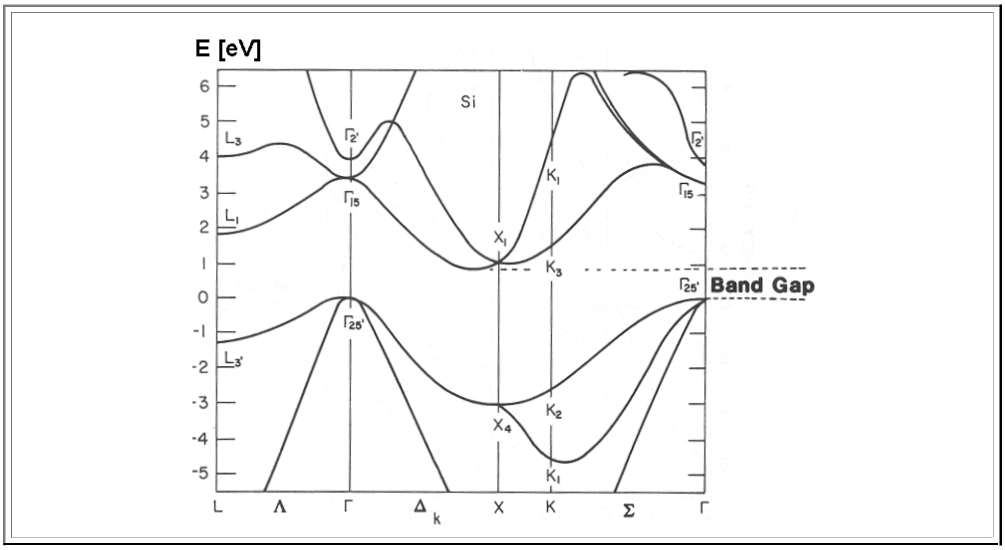
Contemplate this picture a bit and then ask yourself:

  - Do I find this picture alarming ? ("Gee, if even the most simple situation produces such a complicated structure, I'm never going to understand it)
  - Do I find this picture exciting? ("Gee, what a wealth of information one can get in a simple diagram if you pick a smart way of representation").

- Yes, it is a bit confusing at first. But do not despair: If you need it, if you work with it, you will quickly catch on!

It is standard praxis to join the single diagram at appropriate points and to draw band diagrams by showing two branches starting from **Γ** to major points and to continue from there as already practiced above.

- The band diagram of **Si**, e.g., then assumes its standard form:



  - The indexing of the major points in the Brillouin zone is more complex than described so far – it is more than just a band index. This reflects the fact that there is no unique choice of the **Γ** point, or that the the band structure allows certain symmetry operations without changing. The indexing follows rules of group theory displaying the symmetries, but shall not be described here.
- The band structure as shown in this standard diagram contains a tremendous amount of information; at this level it is, e.g., evident that:
  - **Si** has a band gap of about **1 eV**.
  - **Si** is an indirect semiconductor because the maximum of the valence band (at **Γ**) does not coincide with the minimum of the conduction band (to the left of **X**).
- There is, however, a lot more information encoded in this diagram, as we will see later.
- Of course, the question remains how the band structures of real-world materials can be obtained. However, concerning both measurementes and calculations, this is a rather involved subject of its own; we do not treat it here.
  - To get at least a coarse feeling about how involved such calculations are, you may have a look at some really advanced module where the theoretical basics and the available software are presented.