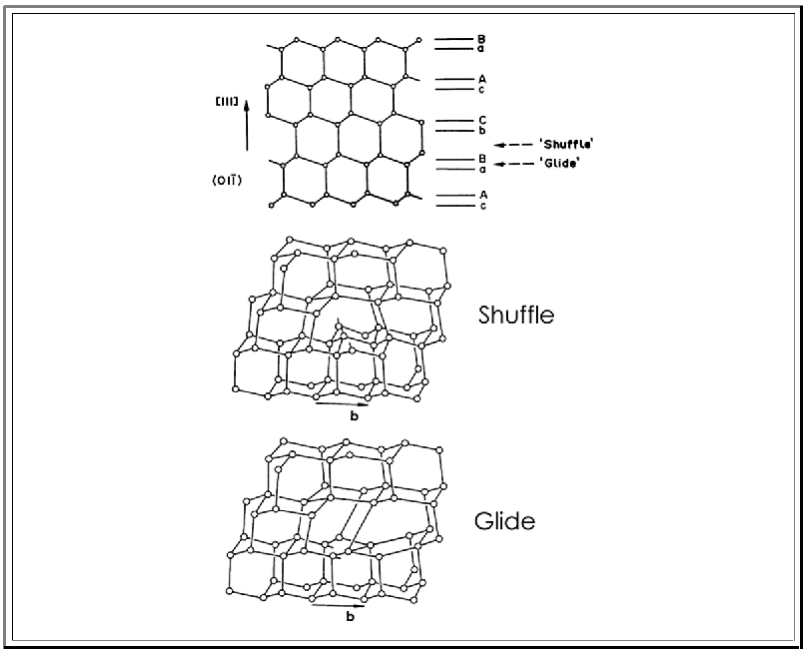
5.4.3 Some Dislocation Details for Specific Lattices

Some Specialities in fcc Lattices

- **Lomer–Cotrell** and **stair-rod** dislocations
  - Lets look at the reaction between two perfect dislocations on different glide planes which are split into Shockley partials, e.g. with the (perfect) Burgers vectors
    $\boldsymbol{b}_1 = a/2[-1,1,0]$ on the **(111)** plane
    $\boldsymbol{b}_2 = a/2[101]$ on the **(–1,1,1)** plane
  - If you have not yet produced your personal Thompson tetrahedra - now is the time you need it!
  - The two Shockley partials meeting first will always react to form a dislocation with the Burgers vector

$$\boldsymbol{b}_{LC} = \frac{a}{6}[011]$$

  - Use your Thompson tetrahedron to verify this!
- This is a *new type of Burgers vector*. A dislocation with this Burges vector is called a *Lomer-Cotrell dislocation*.
  - A Lomer-Cotrell dislocation now borders *two* stacking faults on two different **{111}** planes, *it is utterly immobile*.
  - The total structure resulting from the reaction - a Lomer-Cotrell dislocation at the tip of two stacking fault ribbons bordered on the other side by Shockley partials - is called a **stair-rod dislocation** because it is reminiscent of the "stair-rod" that keeps the carpet ribbons in place that are coming down a stair. What it looks like is shown in the link.
- It is clear that this is a reaction that must and will occur during plastic deformation. Since it makes dislocations completely immobile, it acts as a **hardening mechanism**; it makes plastic deformation more difficult.
- Another speciality in **fcc**-crystals, which would never occur to you by hard thinking alone, are **stacking fault tetrahedra**.
  - Stacking fault tetrahedra are special forms of point defect agglomerates. Lets see what the are and how they form by again looking at low energy configurations:
- Frank partials bonding a vacancy disc have a rather high energy (**b = $a/3$ [111]**, $b^2 = a^2/3$) compared to a Shockley partial ($b^2 = a^2/6$) or Lomer-Cotrell dislocation ($b^2 = a^2/18$), which also can bound stacking faults. Is there a possibility to change the dislocation type?
  - There is! Imagine the primary stacking fault to be triangular. Let the Frank partial dissociate into a Lomer-Cotrell dislocation and a Shockley partial which can move on one of the other **{111}**-planes intersecting the edge of the triangular primary stacking faults. (If you do not have a Thompson tetrahedra by now, it serves you right!)
  - Let the Shockley partials move; wherever they meet they form another Lomer-Cotrell dislocation. If you keep them on other triangular areas, they will finally meet at one point - you have a tetrahedron formed by stacking faults and bound by Lomer-Cotrell dislocations; the whole process is shown in the link.
  - If this seems somewhat outlandish, look at the electron microscopy pictures in the link!
- Next, lets look at slightly more complicated **fcc**-crystals: the **diamond structure** typical not only for diamond, but especially for **Si**, **Ge**, **GaAs**, **GaP**, **InP**, ... Now we have *two* atoms in the base of the crystal, which makes things a bit more complicated.
  - First of all, the extra lattice plane defining an edge dislocation may now come in *two* modifications called "**glide**"- and "**shuffle" set**, because the inserted half-plane may end in two distinct atomic positions as shown below. The properties of dislocations in semiconductors - not only their mobility but especially their possible states in the bandgap - must depend on the configuration chosen.



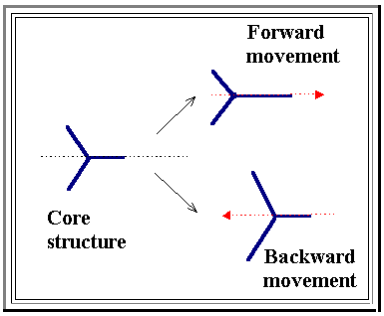
- Which configuration is the one chosen by the crystal? It is still not really clear and a matter of current research.

Some Specialities in bcc Lattices

- The basic geometry in **bcc** lattices is more complicated, because it is not a close-packed lattice.
  - The smallest possible *perfect* Burgers vector is

$$b_{bcc} = \frac{a}{2}\langle 111 \rangle$$

  - Glide planes are usually the most densely packed planes, but in contrast to the **fcc** lattice, where the **{111}** planes are by far most densely packed, we have several planes with very similar packing density in **bcc** crystals, namely **{111}**, {**112}** and **{123}**.
  - This offers many possibilities for **glide systems**, i.e. the combinations of possible Burgers vectors and glide planes. Segments of dislocations, if trapped on one plane may simply change the plane (after re-aligning the line vector in the planes).
  - Stacking faults (and split dislocations) are not observed because the stacking fault energies are too large.
  - But the core of the dislocations, especially for screw dislocations, can now be extended and rather complicated. Screw dislocations in **<111>** directions, e.g., have a core with a threefold symmetry. This leads to a basic asymmetry between the forward and backward movement of a dislocation:



  - Imagine an oscillating force acting on a **bcc** metal - **Fe** for that matter. The screw dislocation will follow the stress and oscillate between two bowed out positions. As long as the maximum stresses are small compared to the critical stress needed to induce large scale movement, the process should be completely reversible.
  - However, due to the asymmetry between forwards and backwards movement, there is a certain probability that once in a while the screw dislocation switches glide planes. It then may move for a large distance, inducing some deformation, In due time, things change irreversibly leading to a sudden failure called "**fatigue**".
  - This is only *one* mechanism for fatigue and only serves to demonstrate the basic concept of long-time changes in materials under load due to details in the dislocation structure of materials.