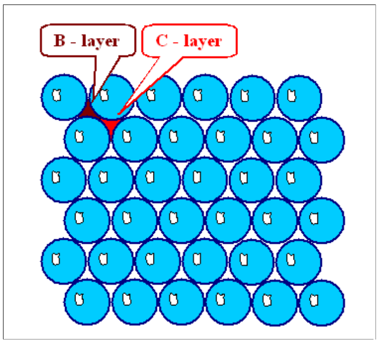
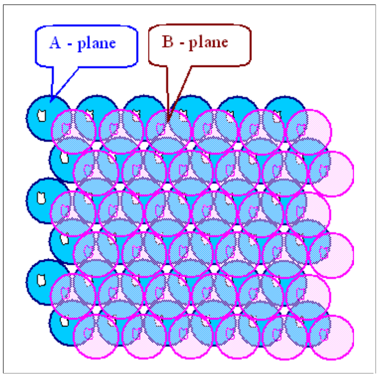
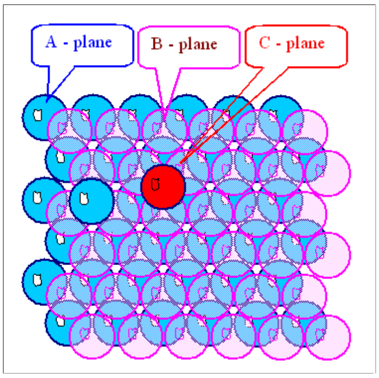
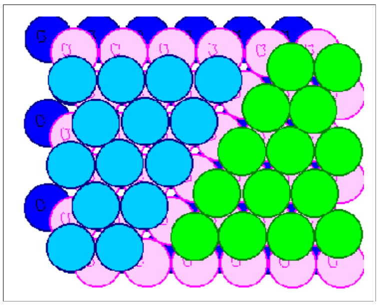
5.4 Partial Dislocations and Stacking Faults

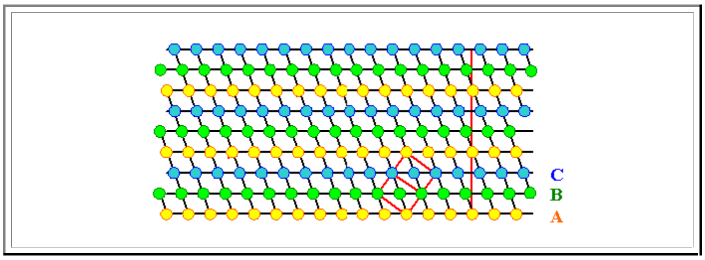
5.4.1 Stacking Faults and Close Packed Lattices

Stacking Faults and Frank Dislocations

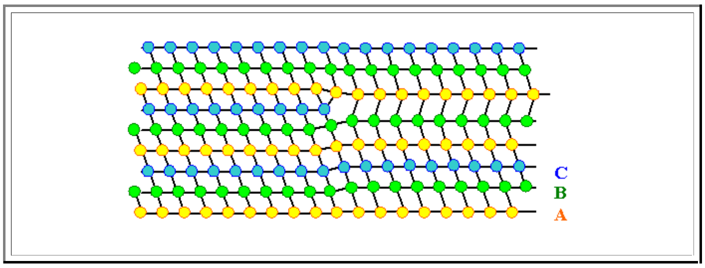
- Let's consider a close packed lattice, and look at the close packed planes.
  - In a simple model using perfect spheres we have the following situation:

	We take the blue atoms as the base plane for what we are going to built on it, we will call it the "**A - plane**".
	The next layer will have the center of the atoms right over the depressions of the **A** - plane; it could be either the **B** - or **C** - configuration.
	Here the pink layer is in the "**B**" position
	If you pick the **B** - configuration (and whatever you pick at this stage, we can always call it the **B** - configuration), the third layer can either be directly over the **A** - plane and then is also an **A** - plane (shown for one atom), or in the **C** - configuration.
	If you chose "**A**"; you obtain the **hexagonal close packed lattice** (***hcp***), if you chose "**C**", you get the **face centered cubic lattice *(fcc)***
	You can't have it both ways. If you start in the **C** position somewhere (in the picture the green atoms) and on the **A** position somewhere else (light blue), you will get a problem as soon as the two layers meet.
	For varieties sake, and to be able to distinguish the layers better, the bottom **A** layer here is in dark blue.

- The stacking sequences of the two close-packed lattices therefore are
  - **fcc**: **ABCABCABCA...**
  - **hcp**: **ABABABA...**
- Looking at this sequences in cross-section is a bit more involved; it is best done in a **<110>** projection of the **fcc** lattice

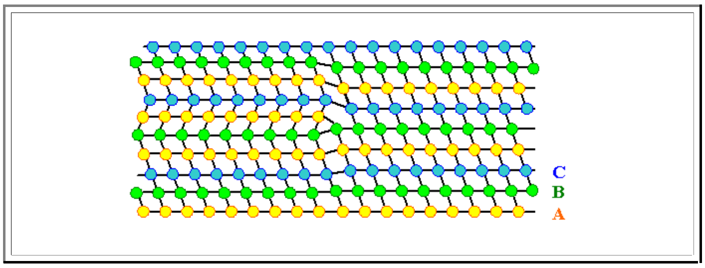


- Planes with the same letter are on lines perpendicular to the **{111}** planes, as indicated by thin black lines.
- The projection of the elementary cell is shown with red lines.
- We now remove *parts* of a horizontal **{111}** plane - e.g. by agglomeration of vacancies on that plane - it shall be a **C**-plane here.



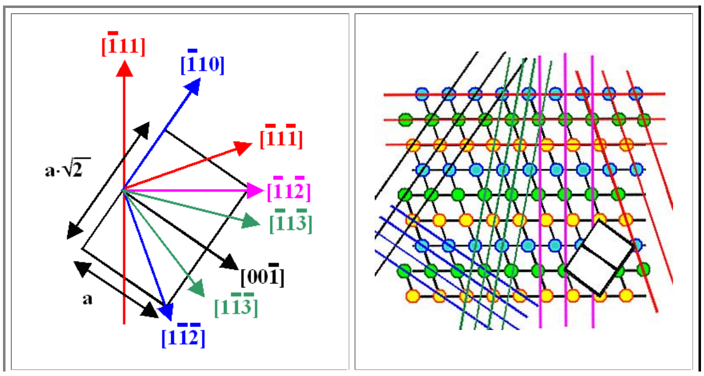
- Now **A** and **C**- planes become neighbors and relax into the configuration shown.
- We produced a **stacking fault** because the stacking sequence **ABCABCA..** has been changed to the faulty sequence
  ABCABABCA...
  The stacking fault is between the large letters.
- Stacking faults by themselves are simple two-dimensional defects. They carry a certain **stacking fault energy** γ; very roughly around a few **100 mJ/m^2**.
- The disc of vacancies obviously is bordered by an *edge dislocation*. What is the Burgers vector of this dislocation? We shall see farther down.

If we do not condense *vacancies* on a plane, but fill in a disc of agglomerated *interstitials*, we obtain the following structure



- The stacking sequence **ABCABCA...** again is faulty; it is now **ABCABACABCA...** .
  The stacking fault is between the large letters.
- This is a *different kind of stacking fault* than the one from above.
- For historical reasons, we call the stacking fault produced by vacancy agglomeration "**intrinsic stacking fault**" and the stacking fault produced by interstitial agglomeration "**extrinsic stacking fault**".
- The extrinsic stacking fault also seems to be bordered by an edge dislocation. Again, what is the Burgers vector?

In order to determine the Burgers vector of the apparent dislocations bordering the stacking faults, we must do a Burgers circuit *or* use the Volterra definition. For this we must first be clear about the directions in the chosen projection. This is shown below.

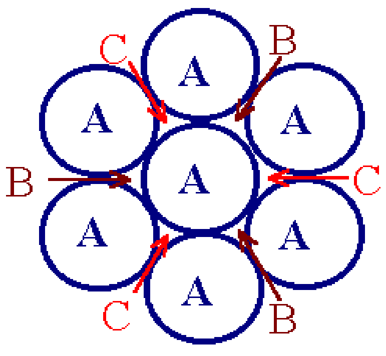
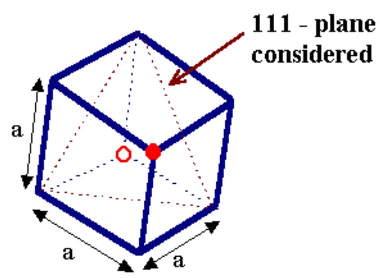
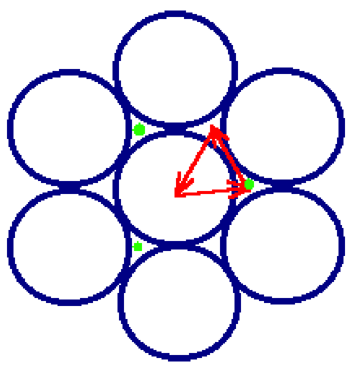


Directions in the **<110>** projection shown for the elementary cell traced out on the right or above	Traces of the (color-coded) *planes* (right angle to direction) in the **<110>** projection and the elementary cell.

- From a Burgers circuit or from a Voltaterra cut, we obtain the same result (Try it! It is easier in this case to hop from atom to atom (instead from lattice point to lattice point); start at the stacking fault).
  - The Burgers vector of these dislocations is ***b* = ± a/3 <111>** - *and this is not a translation vector of the* ***fcc*** *- lattice*! Do not, at this point, forget the distinction between lattice and crystal!
  - Dislocations with Burgers vectors of this type are called **partial dislocations**, or more correctly, **Frank** partial dislocations, or simply **Frank dislocations**.
- This brings us to a general **definition**: Dislocations with Burgers vector that are *not* translation vectors of the lattice are called *partial dislocations*. They must by necessity border a two-dimensional defect, usually a stacking fault.
  - This can be verified with the **Volterra construction** if we add one element: Make a cut in a **{111}** plane and shift by **a/3<111>** perpendicular to the plane. The element added is that we now include shift vectors that are *not* translation vectors of the *lattice*, but vectors between *equivalent positions* of the *atoms*.
  - Partial Burgers vectors and stacking faults thus may exist if the packing of atoms defining the crystal has additional symmetries not found in the lattice. Check this advanced module for an elaboration.
  - As stated in the definition of the Volterra cut-shift-weld procedure, you now must add or remove material. The total effect is the creation of a Frank partial along the cut line and, by necessity, a stacking fault on the cut part of the **{111}** plane.
- We also see now that the primary defects which are generated by the agglomeration of intrinsic point defects in **fcc** lattices are small "**stacking fault loops**".

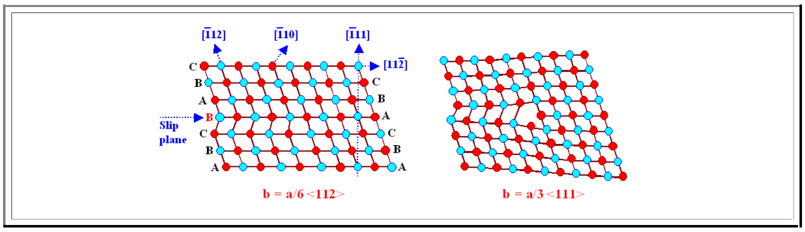
Shockley Dislocations

- Now we may ask a question: Can we produce stacking faults *without the participation of point defects*? Indeed, we may - use the Volterra definition to see how:
  - Make a cut on a **{111}** plane, e.g. between the **A**- and **B**-plane.
  - Move the **B**-plane so it is now in a **C**-position. No material must be removed or added.
  - Weld together: You now have the stacking sequence **ABCACABCA...** instead of **ABCABCA..**, i.e. you produced the stacking sequence of an *intrinsic* stacking fault.
- The vector of the shift must be the Burgers vector of the partial dislocation resulting from this operation as the boundary of the intrinsic stacking fault. This shift vector can be seen by projecting the elementary cell on the close packed **{111}** plane where we did the cut.

		
The displacement vectors for producing stacking faults with the Volterra construction. We have all vectors pointing from one "dent" to a neighboring one.	The directions in the **{111}** plane. If you superimpose the two red circles, you have the projection shown on the left.	Each one of the red vectors would move a **{111}** plane from an A-position to a **B** position (marked by a green dot).

- The relevant displacement vectors are of the type ***b* = a/6<112>**. (Check it! It's good exercise for getting used to lattice projections). Dislocations with this kind of Burgers vector are called **Shockley partial dislocations**, Shockley dislocations, or simply **Shockley partials**.

- In our **<110>** projection, Shockley and Frank partials look like this (after a picture from "Hull and Bacon"). The pictures are drawn in a slightly different style, to make things a bit more complicated (get used to it!)



- You can't quite see the Shockley dislocation? Well, neither can I. But it is time to get used to the fact that not all dislocations are edge dislocation, clearly visible in schematic drawings. We will encounter dislocations that are far weirder and almost impossible to "see" in a drawing, or hard to draw at all. But nevertheless they exist, possess a stress- and strain field described by the formulas from before, and are just the real world inside crystals.

By now you are wondering if these partial dislocations are an invention of bored professors? *Well, they are not!* They are more or less the *only* kind of dislocations that really exist in **fcc** crystals (and some others)!

- The reason for this is that perfects dislocations (with a Burgers vector of the type **a/2<110>**, i.e. a lattice translation vector) will *dissociate to form partial dislocations*. This is one kind of a possible reaction involving partial dislocations, which we are going to study in the next subchapter.