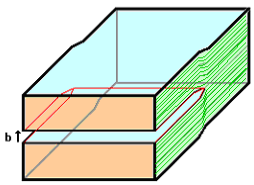
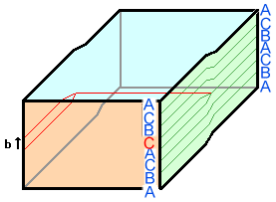
Science

2. The Reality

Partial Dislocations

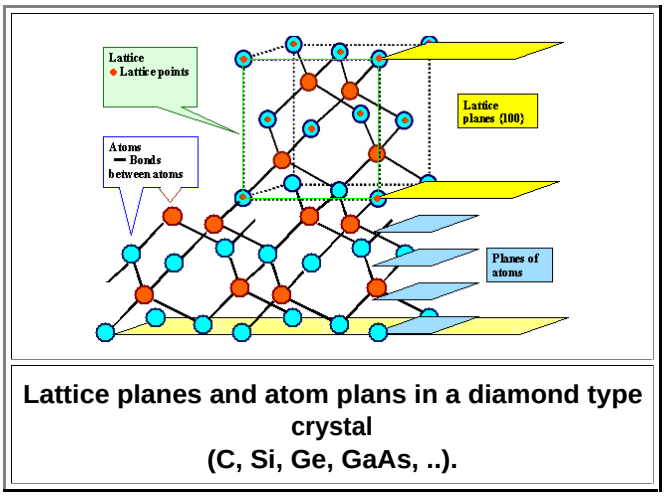
In the first part we have not looked at the dislocations produced when the shift has a component perpendicular to the cut plan. Let's do that now - and be prepared for some mind-boggling results.

- Here is the way to do it:

	**Recipe for lattices:** Cut and move upwards a *translation vector* of the lattice. Fill in the material needed. **Complication for crystals:** Imagine that this is a simple fcc crystal (e.g. aluminum (Al)) and that the faint green lines at its side denote the hexagonally densely packed atomic layers on the {111} planes of the crystal. Then you must insert *three* of those atomic layers to make a *perfect* dislocation!
	Let's *not* do this Let's cut and move upwards just *1/3 of the shortest possible lattice translation vector*. Then only *one* atomic layer needs to be filled in. But now you have a problem! You generated a stacking fault.
Making a Frank dislocation	

Let's look at that a bit more closely. First we just do the simple thing of cutting and moving the right distance, i.e. a lattice translation vector, perpendicular to the cutting plane.

- After the cut (upper figure) we push the two halves apart by the "right" Burgers vector as shown. That necessitates to fill in lattice points and therefore also atoms now.
  That's a point where the distinction between lattice and crystal might cause considerable complications. Depending on the geometry, filling in *one* lattice plane might mean to fill in *several* atomic planes. In our example we need to fill in three planes of atoms, the whole stacking sequence **ABC**.
- To make that a bit clearer, let's look at an example for a diamond kind of *crystal* (which is based on the fcc *lattice*).



Lattice planes and atom plans in a diamond type crystal
(C, Si, Ge, GaAs, ..).

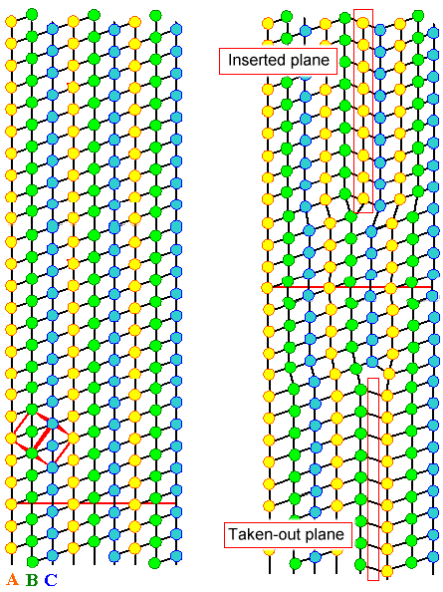
- Well, taking into account this little problem, we fill in as many atomic layers as needed and produce a simple *perfect* edge dislocation once more. Boring.

So how about filling in just *one* atomic layer? That implies that we don't move the cut part up by a full translation vector after the cut but only by a *partial* one. For staying as simple as possible, we *only consider fcc lattices* and crystals now.

- Let's cut along one of the densely packed planes (or a {111} plane) of a fcc lattice / one-atom-base crystal. The stacking sequence of the *atomic planes* is **ABCABC...**; it is indicated in the bottom part of the figure above. If we make the cut and then move up just **1/3** of the length of a proper lattice translation vector, we have precisely the space to insert exactly *one* atomic layer. Now between an **A**-layer and **B**-layer you can only insert a **C**-layer, between a **B**-layer and **C**-layer only an **A**-layer fits, and so on. If we do that we get something that looks very much like an edge dislocation but with a **stacking fault** on one side!

We have made a **partial dislocation** in this way. The particular kind we made in fcc crystals is called a **Frank** dislocation; its Burgers vector is $\underline{\boldsymbol{b}}_{\mathbf{Fr}} = \mathbf{a/3}\langle\mathbf{111}\rangle$

- Of course, we can do the same thing by moving the other way and *taking out* one atomic layer. What one gets is shown below.



Frank partial dislocations and stacking faults in a fcc lattice / crystal.

On the left is the perfect lattice / crystal. The unit cell is indicated and the red line denotes the direction along which you count the stacking sequence. On the right, one extra plane has been inserted or removed, generating a Frank dislocation with a stacking fault on one side.

- Note that a Frank partial dislocation cannot move without the help of point defects. Movement on its formal glide plane (the plane containing Burgers and line vector) would require that the stacking fault moves, too. That necessitates the movement of all the atoms in the stacking fault which simply won't happen.

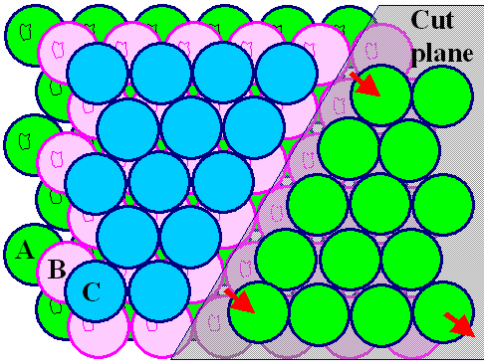
It is easy to insert or to remove atomic planes with a drawing tool. But how is the crystal doing it?

- Well, as you know from the backbone, by condensing vacancies or self-interstitial atoms on one plane. In the backbone, however, I have never mentioned the word "*partial dislocation*" for good reasons.
  Here, it becomes clear that a stacking fault that doesn't end at the surface or some internal interface, by needs must be bound by a partial dislocation.
  When point defects agglomerate on a plane they start small and thus cannot be bound by interfaces all around. They typically form a dislocation loop enclosing the stacking fault. The dislocation must be a Frank partial dislocation (with a Burgers vector of $\underline{\boldsymbol{b}}_{\mathbf{Fr}} = \mathbf{1/3}\ \langle\mathbf{111}\rangle$). Once a small dislocation loop of this kind has formed (with the usual nucleation problems), it could easily gobble up all the excess point defects, growing in diameter by doing so.
- So far I only gave you grain boundaries as "sinks" for point defect, as places where they could disappear. Now we also have the nucleation and growth of a dislocation loop enclosing a stacking fault as a way to get rid of unwanted point defects.
  If excess point defect are around, starting such a loop is great for nirvana. You gain free energy in removing them, and the (energy) costs of having small dislocation loops instead of lots of individual point defects my well be worth it. But there is a problem. The problem is that the energy of such a dislocation loop increases rapidly as the

diameter d_{loop} grows. The energy contained in the stacking fault grows with the area enclosed, i.e. with d^2_{loop} and to this you must add the energy of the Frank dislocation that grows with its length, i.e. d_{loop}. Above a critical size the loop energy gets too large and it is no longer a good investment for removing point defects

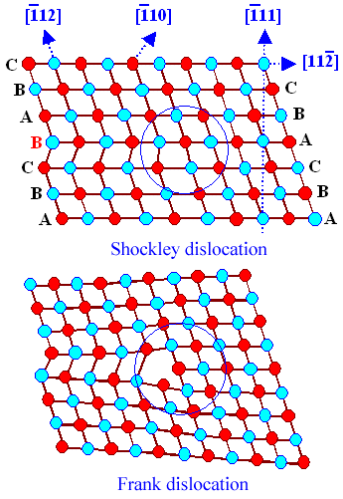
Can we do something about that? Well, yes - also I doubt that you and most others of my readers could come up with the trick for that. The crystal, as always, just does it. The key is to find *another* kind of partial dislocation that is connected with a stacking fault.

All we need to do for this is to get smart about the "cut-and-shove" procedure. Just cut along the densely packed **ABCABC...** planes, e.g. between a **B** and **C**-plane as shown below, and shove the **C**-plane into an **A**-plane position as shown. Everything above the **C**-plane moves, and you get a stacking sequence of **ABCAB**A**BCABC..**. Wherever your cut ends, you have a partial dislocation called a **Shockley dislocation** with its Burgers vector in the densely packed planes.
Geometry reveals that the Burgers vector $\underline{\boldsymbol{b}}_{Sh}$ must be of the $\underline{\boldsymbol{b}}$ **= a/6**<**112**> type.



Making a Shockley partial dislocation with a stacking fault.

Shockley dislocations are not that easy to draw or recognize; the figure below shows that. But pictures mean nothing, it is the stress and strain field that "makes" a dislocation.



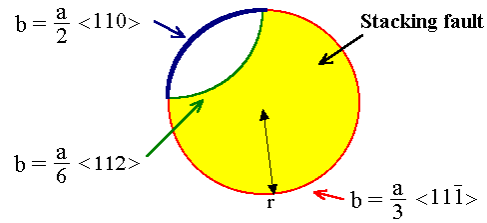
Frank and Shockley partial dislocations with stacking faults on one side

The dislocation cores are inside the blue circles. While the Frank dislocation looks like a proper edges dislocation, the Shockley dislocation does not betray itself in such an obvious way.

"Is that an exercise in crazy geometry or what?" you might be asking now. No, it is not. The trick is that

- A Shockley and a Frank dislocation can combine into a perfect dislocation à la **a/6<112> + a/3<1,1,-1> = a/2<110>**.
- The reverse is also true. A Frank dislocation can split into a Shockley dislocation and a perfect dislocation.

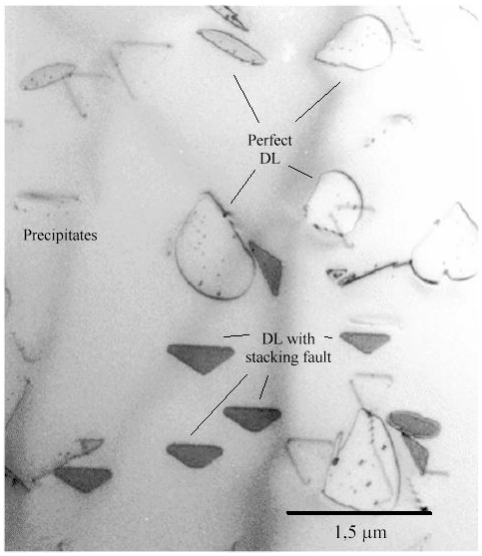
- An that's what the Frank dislocation bordering a point-defect stacking-fault disc *will* do if the dislocation loop plus enclosed stacking fault gets too big! here is a schematic figure:



Defaulting a dislocation loop with stacking fault by moving a Shockley dislocation across it.

- The "Frank" splits into a "Shockley" and a perfect dislocation in a small part of its length, The Shockley then sweeps out across the loop, removing the stacking fault. What is left behind is a dislocation loop bound by a perfect dislocation that can move wherever it likes because it doesn't have to schlepp a stacking fault around.

If you think that is is rather academic, think again. The following pictures might help:



Dislocation loops with stacking faults, unfaulted loops, and precipitates in gallium phosphide (GaP) after zinc (Zn) diffusion.

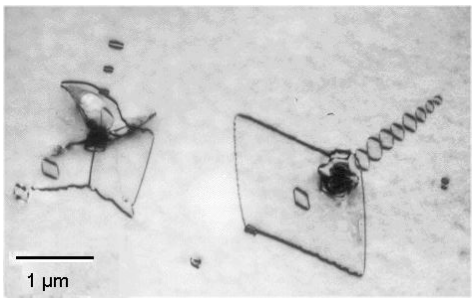
Source: PhD thesis Ch. Jäger, Mikrostrukturanalytik, University Kiel

- Gallium phosphide (GaP) is a key material for optoelectronics. Certain processing leads to the whole chain of point defect agglomeration: faulted Frank-type dislocation loops, unfaulting with Shockley partials, formation of perfect dislocation loops, moving of the perfect dislocations, interaction, formation of a perfect dislocation network.
  This is not good!
  The perfect dislocations start moving, drawing out the loop, encounter each other, and start to form dislocation networks throughout the formerly nearly dislocation-free single crystal. This is already occurring in the lower right-hand corner. At this point you can just as well throw away the crystal or the devices made from it, they won't work anymore.

There are plenty more examples but I will leave it at that. What we need to realize is:

There are mechanisms to generate "big" defects (e.g. lots of dislocations)
from point defects!

- The mechanism above is not the only one. I will give you one more example because the picture is so enticing:



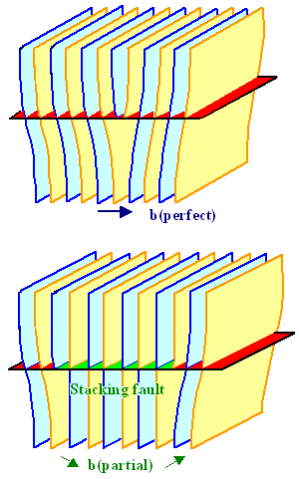
Dislocations loop generation in silicon (Si) by SiO_2 precipitates .

Source: My friends H. Strunk and B.O. Kolbesen

- Small silicon dioxide (SiO_2) precipitates form during first processing for microchips in otherwise extremely perfect silicon single crystals. They are actually wanted for certain reasons, and that's why a small amount of oxygen (around 10 ppm) is left in the crystals.
  What is *not* wanted is that those precipitates (the blackish blobs) start to generate dislocations in the form of a succession of small loops that, God forbid, might grow, interact and fill the crystal with dislocations.
- I'll leave it at that. Now let's look at the difficult stuff.

Split Dislocations, Kinks, Jogs - And What Really Happens

- Once again, our cut-and-shove way of making a (perfect) dislocation was for a *lattice* . If we look at a *crystal*, things get more complicated. As an example, let's cut through the simplest crystal possible: fcc with just one atom per lattice point. The cut plane shall be the most densely packed {111} plane, and we shove for a simple edge dislocation.
- Looking at the result in a certain projection, we see that *two* atomic planes actually end for each *lattice* plane.

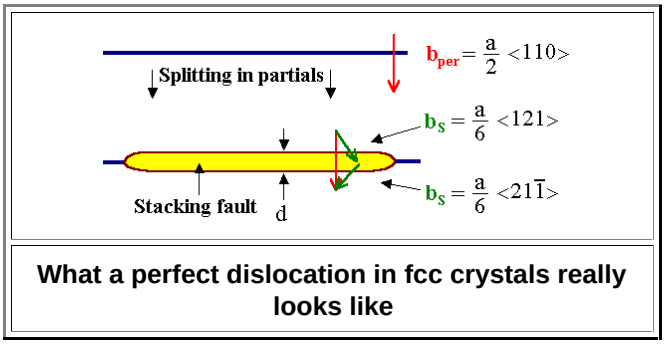


Result of cut-and-shove for a simple edge dislocation in an fcc crystal in some suitable projection.
Two atomic planes end - but only *one* lattice plane (you can take either the blue or the yellow plane to symbolize just lattice planes).
It looks suspiciously like *two* dislocations next to each other, and that's what they actually are: two partial (Shockley) dislocations.

The forces between the two partials are repulsive, and that's why they move apart. In the figure the two partial dislocations have moved apart - and pulled out a stacking fault between them. The simple perfect edge dislocation has now split into two partial dislocations with a stacking fault in between.

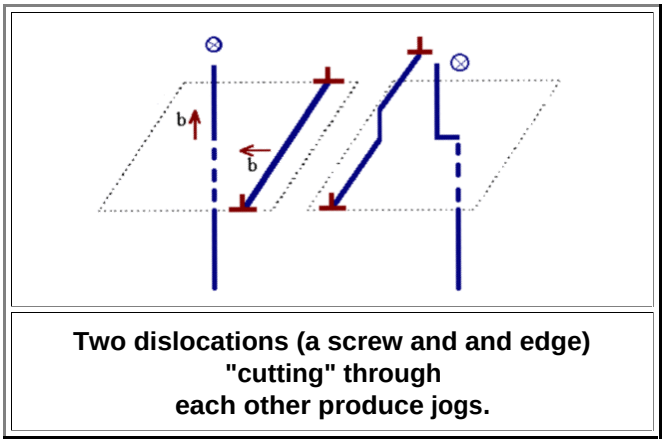
How a perfect dislocation splits into partial dislocations

- To make a long story short: there is no such thing as a simple perfect dislocation in fcc crystals. They are always (well, almost always) split into two partial dislocations with a stacking fault in between.
  - The two partials at the core of a perfect dislocation repel each other and thus move apart, the stacking fault in between, like a rubber sheet pulls them back. It follows that there is some equilibrium distance where the forces cancel, typically some ten nanometers. It looks like this:



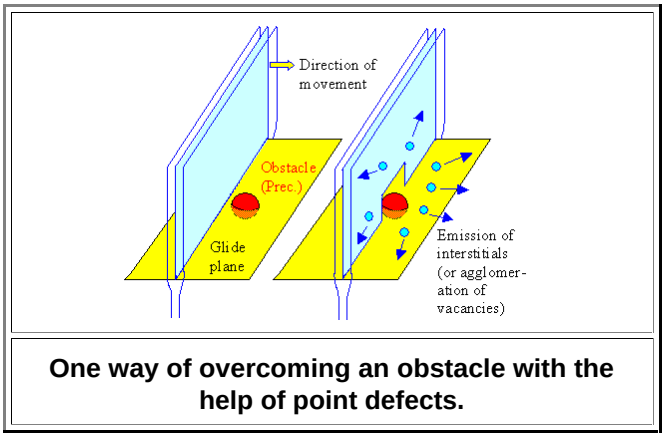
What a perfect dislocation in fcc crystals really looks like

  - Instead of a simple dislocation line we actually have a *ribbon*, formed by two partial dislocations on the outside and a stacking fault in between.
- Bad enough, so let's not linger but go for broke.
  What happens if two arbitrary dislocations with dislocation lines (or ribbons) running in *different* directions move across each other? Well that's actually simple to answer, look a the figure below.



Two dislocations (a screw and and edge) "cutting" through each other produce jogs.

  - If a dislocation moves, one part of the crystal slips one Burgers vector with respect to the other part. In the figure above it is made clear what happens: both dislocation lines line are no longer straight but have a "jog", a displacement by one Burgers vector of the other dislocation.
    Note that the jog in the screw dislocations has "edge" character, meaning that this short part of the dislocation has just *one* defined glide plane in contrast to the rest of the "screw". That will make the movement of the screw more difficult.
- Now let's look what happens if an edge dislocation encounters a small obstacle, i.e. a small precipitate.



One way of overcoming an obstacle with the help of point defects.

- In the left part of the figure the edge dislocation is stuck because it cannot overcome the obstacle (a rather small precipitate in this example). All it needs to do to get unstuck is to emit a bunch of self-interstitials. That will "eat" away that part of the extra lattice plane that is stuck and thus allow bypassing the obstacle. If vacancies happen to be around, they can also do the job by agglomerating where it is needed.
  The dislocation now contains what we call a "**kink**", and in acquiring this kink it has "**climbed**", i.e. performed (in parts) a movement off its glide plane.

Two examples out of a large number. Just consider what would happen in the two situations above if the dislocation types would be different. Or if the orientations of the "actors" is different. If you can predict (without further help) what a screw dislocation will look like after it "climbed" around an obstacle, I will make you an honorary graduate of my "defects" class.
Then consider that all dislocations are actually a split into two partial dislocations. And so on. And so forth

- Not to forget: Consider if there are *other ways* besides using point defects to get around obstacles (there are). And how all that might depend on the temperature. And....

Enough. You get the idea. It ain't all that easy to figure out in detail what happens if you bang a crystal with a hammer, generating dislocations and make them move.
And so far we looked only at *fcc crystals*!

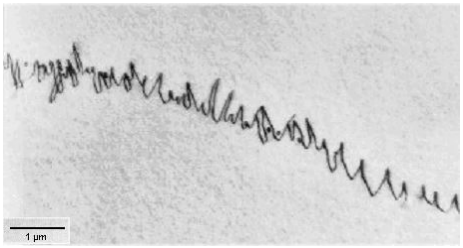
- Considering that we want to understand iron and steel, typical *bcc crystals*, you might ask me now "How about those? Or hex crystals, while we are at it?"
  My answer is simple "It's considerably worse! Let's not go into it"

Allright, here come the infamous last words:

- As soon as dislocations are doing something, i.e. move in response to stress in the material, their mutual interaction generates a huge mess. The dislocation lines get twisted, bend and mutilated, they produce and / or gobble up point defects, leave back "debris" like small dislocation loops, and so on.
- All this affects how easy it is to move them.
- All of this determines the hardness of your material!

Now the thought for the nightmare:

- The electron microscope picture below shows a dislocation in silicon that has been quite busy. Originally it was a nice and straight screw dislocation. Then it encountered vacancies and interstitials.
  Note that this is a two-dimensional projection of a three-dimensional structure. The dislocation line in three dimensions is rather helix-like. Now comes the questions:
  How do you have to cut with your virtual knife to make such a cut-line?



Dislocation line after busy times.

Source: Courtesy of my friends H. Strunk and B.O.Kolbesen.

- The correct answer is: I have no idea. Nor need I have to have one because I have long since abandoned working with "pictures", virtual knifes, and analogies. A dislocation - any dislocation - has become an entity of its own, described in more abstract quantities or by a bunch of equations if needs be, that do not need "pictures".

Back to **Dislocation Science**

On to

- **1. The Basics**
- **2. The reality**
- **.3. Specialities**