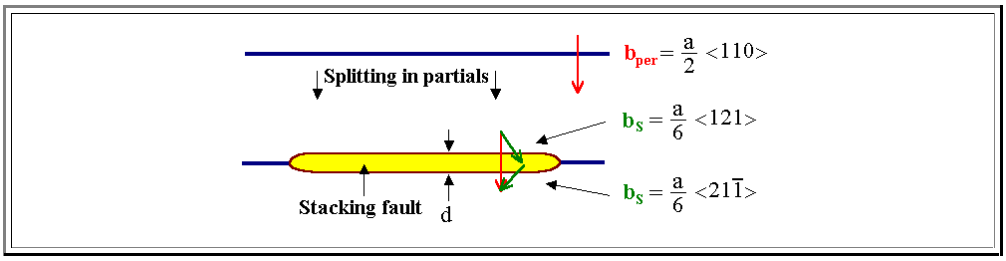
5.4.2 Dislocation Reactions Involving Partial Dislocations

Splitting of Perfect Dislocations into Partial Dislocations

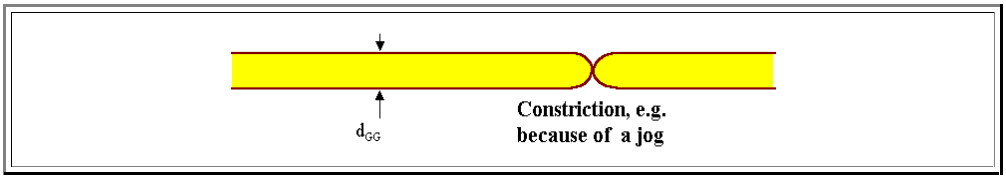
- A perfect dislocation may dissociate into two partial dislocations because this lowers the total energy.
  - The Burgers vector ***b* = *a*/2[110]** may, e.g., decompose into the two **Shockley partials *a*/6[121]** and ***a*/6[2,1,–1]** as shown below.
  - Of necessity, a *stacking fault* between the two partial dislocations must also be generated.



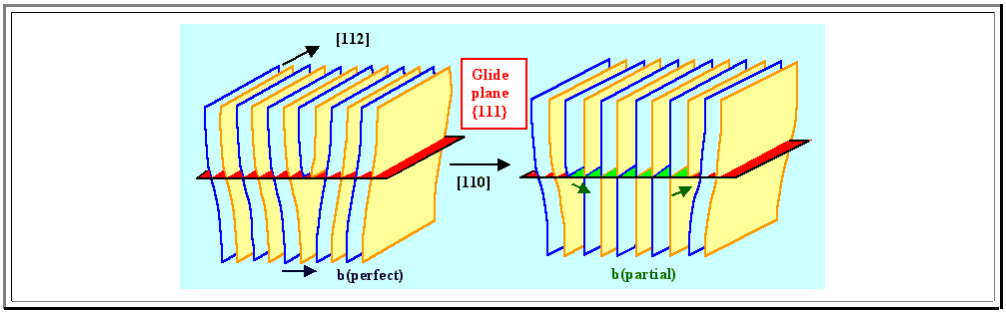
  - You can think of this as doing *two* Volterra cuts in the same plane, each on with the Burgers vector of one of the Shockley partials, but keeping the cut line apart by the distance ***d***. Each cut by itself makes a stacking fault, but the superposition of both creates a perfect lattice.
- Lets balance the energy of this reaction:

Energy of the perfect dislocation	$= G \cdot b^2 = G \cdot (a/2<110>)^2$	$= \frac{G \cdot a^2}{2}$
Energy of the two partial dislocations	$= 2G \cdot (a/6<112>)^2 = 2G \cdot a^2/36 \cdot (1^2 + 1^2 + 2^2)$	$= \frac{G \cdot a^2}{3}$

  - We thus have a clear *energy gain* $-E_{split} = G \cdot a^2$ by having smaller Burgers vectors. This energy gain does not depend on the distance ***d*** between the dislocations.
- But we are not done yet; we have two more energy terms to consider:
  - **1.** The *energy of interaction* $+E_{inter}$; it will be large at short distances. The dislocations repulse each other and the energy going with this interaction is proportional to **1/*d***. Based on this *alone*, the partial dislocations thus would tend to maximize ***d***.
  - **2.** The *energy of the stacking fault* $+E_{SF}$ stretched out by necessity between the two partial dislocations. This stacking fault energy is always $E_{SF} = \gamma \cdot$ **area**, or, taken per *per unit of length* as for the dislocations, $E'_{SF} = \gamma \cdot d$. Based on this *alone*, the partial dislocations thus would tend to minimize ***d***.
- In total we have some energy *gain* by just forming partial dislocations in the first place, but energy *losses* if we keep them too close together, or if we move them too far apart.
- We thus must expect that there is an **equilibrium distance d_{eq}** which gives a minimum energy for the total defect which consists of a **split dislocation** and a **stacking fault**. This equilibrium distance d_{eq} will depend mostly on the stacking fault energy γ; for small γ's we expect a larger distance between the partials.
  - In principle, we can calculate d_{eq} by writing down the total energy, i.e. the sum of the energy gain by forming partial dislocations plus the energy of the interaction plus the stacking fault energy, then find the minimum with respect to ***d*** by differentiation. This is a basic execise, what you will get is $d_{eq} \propto \gamma^{-½}$
- Instead of a a pure one-dimensional defect - our perfect dislocation - we have now something complicated, some kind of ribbon stretching through the crystal. Moreover, this stacking fault ribbon may be constricted at some knots or jogs, and may look like this:



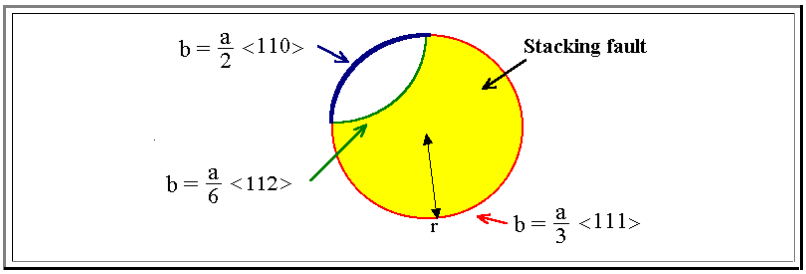
- How would this look in cross-section? We take a picture after "Hull and Bacon"



- It is clear that a dislocation split into *Shockley partials* is still able to glide on the same glide plane as the perfect dislocation; the stacking fault just moves along. It can also change its length without any problems.
- For *Frank type partials* this is *not* true. The loop it usually bounds could only move on its glide cylinder. Changing the length would involve the absorption or emission of point defects.

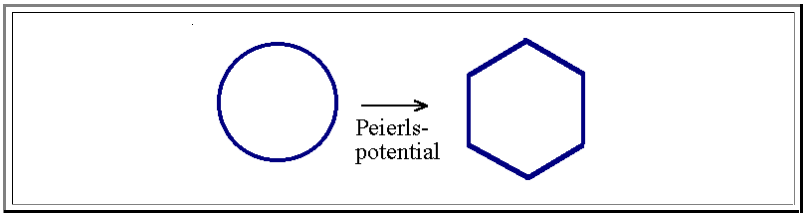
Reactions between dislocation now tend to become messy. You must consider the reaction between the partials and taking into account the stacking fault. However, processes now become possible that could not have occurred before. Lets look at some examples.

- A small dislocation loop formed by the agglomeration of vacancies, that in its pure form cannot add much to plastic deformation, may transmutate into a dislocation loop bounded by a perfect Burgers vector (which in turn may split into Shockley partials) - it is now glissile and can increase its length ad libitum. How does that happen?
- As shown below, the Frank partial bounding the vacancy disc defining the stacking fault has a Burgers vector of the type ***b* = *a*/3<111>**. It then may split into a perfect dislocation with **b = *a*/2<110>** and a Shockley partial with ***b* = *a*/6<112>** (which must lie in the loop plane). The Shockley partial moves across the loop, removing the stacking fault - we have an "**unfaulting**" process. A loop bounded by a perfect dislocation, free to move, is left. The glide plane of the perfect dislocation is not the plane of the loop; the Burgers vector of the perfect dislocation, after all, must have a sizeable component perpendicular to the loop plane in order for the sum of the Burgers vectors to be zero.

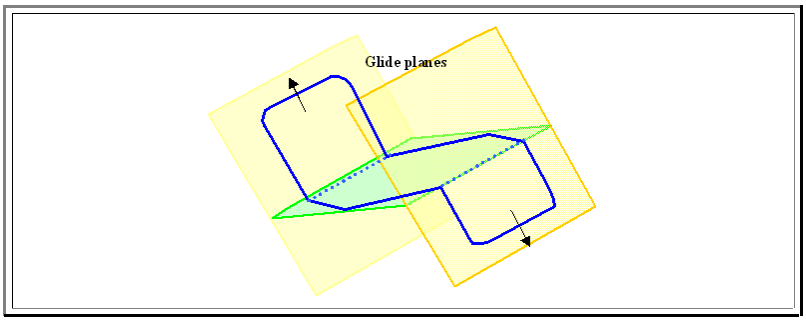


- The Shockley dislocation, once formed, will move quickly over the loop - pulled by the stacking fault like by a tense rubber sheet. The driving force for the reaction is the stacking fault energy: As the loop increases in size because more and more vacancies are added and the radius ***r*** grows, the energy of the loop increases with r^2 due to the stacking fault. However, the line energy of the dislocation only increases with ***r*** no matter what kind of dislocation is bounding the loop.
- There is therefore always a critical radius r_{crit} where a perfect loop becomes energetically favorable.

The perfect loop now feels the Peierls potential, it may try to align the dislocation into the **<110>** directions, always favorable in **fcc** lattices the loop then assumes a hexagonal shape.



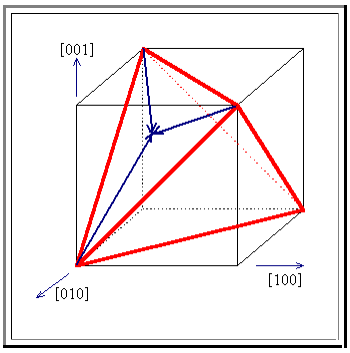
- Now all segments are able to glide. If the resolved shear stress for some segments is large enough, they are going to move, pulling out long dislocation dipoles in the direction of the movement. The beginning of this process may look look this:



- What we have, in summary, is one of the problems of **Si** materials technology:
  - We have an efficient source for dislocation generation by vacancy (or, in **Si**, interstitial) agglomeration in formerly dislocation free crystals! And this is not a theoretical possibility, but reality if you are not very careful in growing your crystals. Many examples are shown in the link.

The Thompson Tetrahedron

- As we have seen, there are now many possible dislocation reactions. In writing down reaction equations, you must use the specific Burgers vector (e.g. ***a*/6[1, -2, 1]**) and not the general type (***a*/6<112>** for the example). This can be cumbersome and is prone to produce errors.
  - Fortunately there is a extremely useful tool for **fcc** lattices to keep the vectors in line: The *Thompson tetrahedron*.
  - The Thompson tetrahedron is simply the tetrahedron formed by the **{111}** planes with consistently indexed planes and edges.



  - If we look at the **{111}**-planes tetrahedron, we see the following connections
    - The *edges* are **<110>** directions, they may be used to represent the Burgers vectors of the perfect dislocations and the preferred direction for the line vectors because of the Peierls potential (red lines).
    - The *faces* are **{111}** planes, they show the positions of potential stacking faults.
    - The Burgers vector of the Shockley partials that may bound a stacking fault of the given **{111}** plane are the vectors running from the *center* of the triangular faces to the corners (blue lines)
    - The Frank dislocations that also can bound a stacking fault, run from the center of the triangular faces to the center of the tetrahedron (not shown).
  - For a "short-hand" description, it is conventional, to enumerate the edges by **A,B,C,D** and the centers of their triangles by **α, β, γ** and **δ**. The relevant vectors than become, e.g., **AB** or **Aγ**.
  - It is a good idea (*really!*) to really build a Thompson tetrahedron - maybe from some stiff cardboard; the link gives the detailed net.