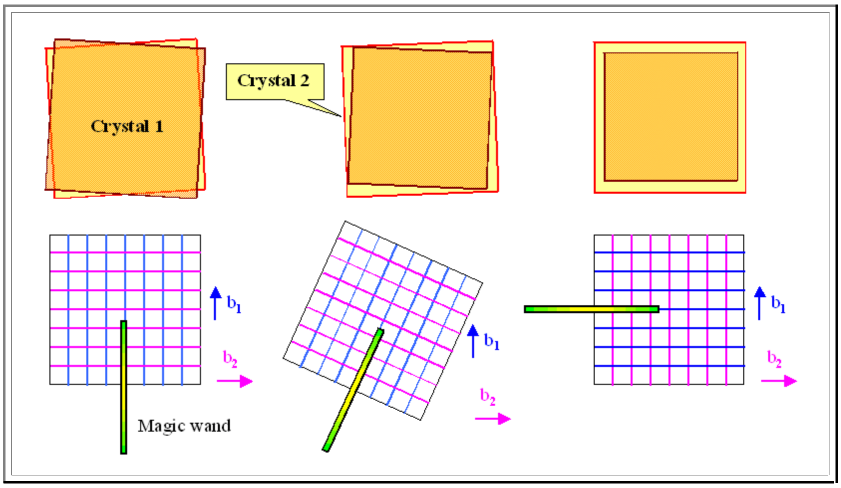
Compliant Substrates

Advanced

- In **1997**, the idea came up to accomodate the stress in a phase boundary arising from the misfit by using existing defects some distance away from the interface which then may not be harmful to the device. In particular, a small-angle grain boundary some **100 nm** away from the phase boundary was found to do the job.
  - The concept is easy to understand on the background of the case studies for small angle twist boundaries discussed before.
  - Lets discuss how you can make a phase boundary *free of misfit dislocations even for misfits **> 10 %*** and layer thicknesses of many **nm**. We will do this in the form of a recipe, giving the ingredients with a brief discussion of what they do.
- Lets assume we want to produce a **GaAs** layer on top of a **Si** substrate (this is something a lot of people would love to do! [1]). The misfit - roughly - is **10 %** so there is no chance whatsoever to produce a misfit dislocation free interface by just depositing **GaAs** on top of **Si**. We do it as follows:
  - Bond two **Si** wafers together with a (twist) misorientation of about **10°** . A small angle grain boundary will form that is identical to the one shown before - except that the spacing of the dislocations will be considerably smaller.
  - Polish off one of the wafers until only a layer with a thickness of a few **100 nm** remains. This is not exactly easy, but state of the art in wafer processing.
- Now you have a **compliant substrate**. Deposit your **GaAs** on top of it and be confident that you have no misfit dislocations in the phase boundary.
- How does this work? On the one hand, the details are none to clear, one the other hand, it is simple. We look at the other hand.
  - Imagine a ***magic wand*** that you can glue to the screw dislocation network in the small angle grain boundary. Now hold your substrate crystal firmly in place, and *rotate the complete dislocation network by **90°***. What then happens is shown below.



  - If you rotate the dislocation network by **90°**, you produce an *edge dislocation network*. Remember that the *Burgers vector* is fixed; it does not depend on the direction of the *line vector* - which is the only vector you change by the rotation.
  - The spacing ***d*** of the dislocation network remained unchanged and it is now exactly the kind of network you need to accommodate differences in lattice constants. Compare the networks in the small angle twist boundary in **{111} Si** with the network in the phase boundary **{111}Si - (hex)NiSi$_2$**. While the networks are identical in geometry, one consists of *screw dislocations*, the other one of *edge dislocations*.
  - In the twist boundary, the misorientation angle was given by (approximating **sin(α)** ≈ α):

$$\alpha = \frac{b}{d}$$

  - For an edge dislocation network, the misfit in lattice constants is simply

$$d = \frac{b \cdot a}{\Delta a}$$

- We thus can now accommodate a misfit of

$$\frac{\Delta a}{a} = \frac{b}{d} = \alpha$$

Wow! An angle of **10^o**, easily within the range of small angle grain boundaries, will have a value of about **0,175** in angular radians and thus corresponds to a misfit of **17.5 %** !!!!

- If this works, we could accommodate huge misfits with no dislocations in the phase boundary. The prize to pay is that we have a dense area of edge dislocations some **100 nm** below the phase boundary. But that may not be detrimental to the electronic or optoelectronic uses you had in mind for your phase boundary.

The question, of course, is: *Does it work?* Especially if your magical wand is at the repair shop? The answers are:

- **1.** Yes **-** it works, at least in principle. But much research and optimization needs most certainly to be done before compliant substrates can be used for products.
- **2.** Your magic wand is supplied by the forces acting on the dislocations as soon as you start depositing the strained layer. These forces will try to rotate the dislocations from screw to edge orientation. So not having a wand is not the real problem.
- However, there is no way to rotate a complete network as a whole. But *patches* of network, separated by a third set of dislocations accommodating steps or some small tilt component as seen in the example, can possibly rotate independent of each other.

Finding out exactly how this can happen (and thus how to optimize it by creating an optimized boundary structure) will be one of the keys for success with this technique.

- This shows to demonstrate that knowing a few things about dislocations may come in handy one day.
- So try it. See if you can figure out how the screw dislocation network can rotate patch by patch by suitable dislocation interactions, involving, maybe, a bunch of additional dislocations as needed, e.g. to accommodate a small tilt component.

1) They actually did it, consult the link!