

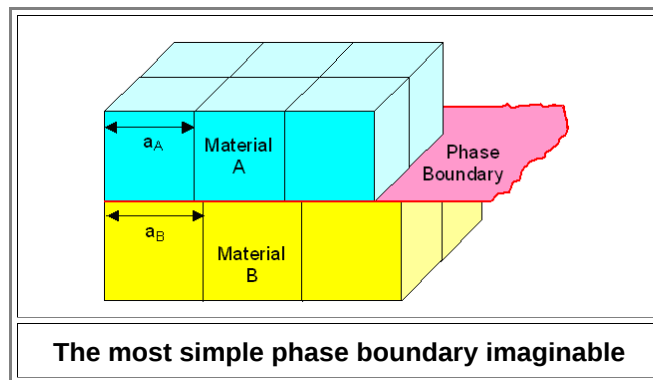
Phase Boundary - Advanced

Advanced

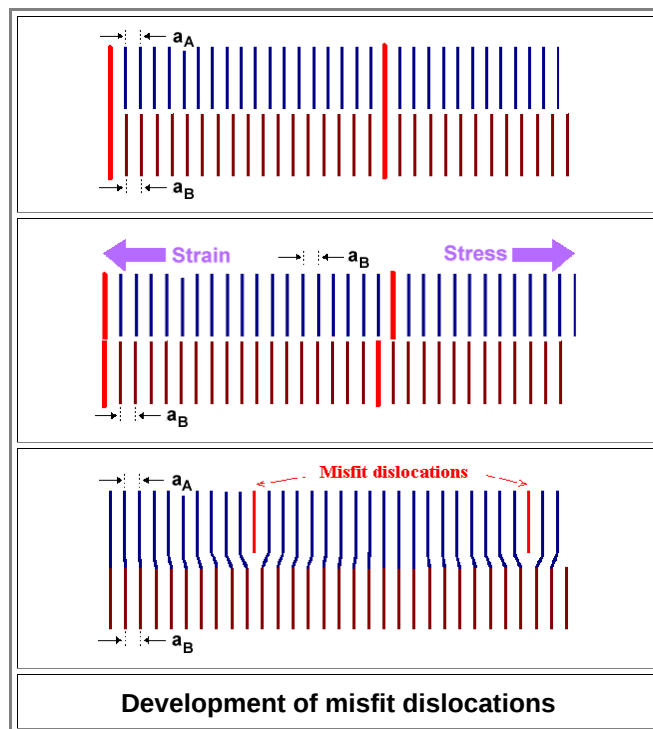
We are going to look at phase boundaries in two ways here. First we look at the general case, after that we consider a very special one.

Dealing with the general case would be quite straight-forward. First, we would acquaint ourselves in great detail with the [science of grain boundaries](#). We would need far more details (including a lot of math with matrices and vectors) than what you will find in the link. Then we would add a lot more complexity, accounting for the fact that the lattices on both sides of the phase boundary are not the same as in the case of a grain boundary. If we would do that - and we most certainly will not - all we would find in the end is that the phase boundary might contain some structures resembling the networks of grain [boundary dislocations](#), just being more complex.

That shall be enough for the general case. Now let's look at a special case of great importance for technology. For that we consider the **most simple** phase boundary imaginable. We will join two crystals of the same kind (cubic, let's say) with no misorientation on a simple plane, for example on one of the planes of the cube as shown below.



Assuming that the atoms in **A** and **B** like each other enough to bond with gusto, what is going to happen? That becomes clear as soon as we redraw the situation above a bit:



Since the lattices put on top of each other don't match (top figure), there simply cannot be a happy atom-by-atom joining across the **interphase** (note the clever spelling!). The crystal must do something about this. To understand its options more easily, let's assume that material **A** is deposited on top of material **B** to some small thickness d_A . In other words, we are looking at "**thin layer technology**", one of the cornerstones of all semiconductor technology. However, we can make the layer as thick as we like in principle, so all bases are covered here. There are exactly two options for the system: substrate **B** and (thin) layer **A**:

● **First option:** Squeeze one lattice in such a way that it will match. This is shown in the middle figure. Some stress needs to be applied to the thin layer in this case, producing the proper strain for matching the lattices. The atoms across the interphase can join now. It is of course the violent mating of atoms across the interphase that produces the stress; nothing needs to be done from the outside.

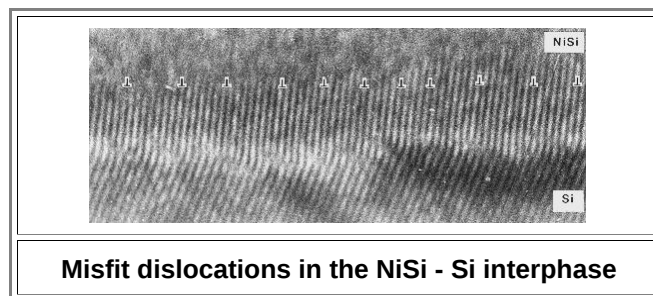
There is a price to pay, however, for all this jolly mating. The upper material in the example is under tensile stress and thus contains some **energy** like a wound-up spring. This energy increases directly with the amount of the misfit **and** the thickness d_A of the layer.

● **Second option:** Introduce **misfit dislocations** as shown in the lower figure. In between these dislocations the lattices can be joined by just a little bending.

Once more there is a price to pay. Dislocations contain energy, and the total cost is proportional to the total length of the dislocations. Since you need more dislocations to accommodate larger misfit, the price increases with the amount of the misfit - but is **not** dependent on the layer thickness d_A .

The consequence of this is clear. If the layer thickness is below some critical value d_{crit} , it is cheaper to squeeze a bit. If the layer thickness is larger than d_{crit} , the system is better off with misfit dislocations.

■ We must expect that misfit dislocations are introduced in an interphase as soon as the critical thickness is surpassed while we deposit the layer. This most certainly (and unfortunately) will happen for all interphases. Here is just one example (another one can be found in [this link](#)):



● It's a hexagonal NiSi lattice on top of the cubic silicon. No problem, just put the NiSi on [{111} oriented](#) silicon. That's why there is a "kink" in the lattice planes.

I like this picture a lot because **I** took it in 1979 **and** it happens to be the first HRTEM picture showing not only misfit dislocations in a phase boundary, but the highest density ever encountered by then.

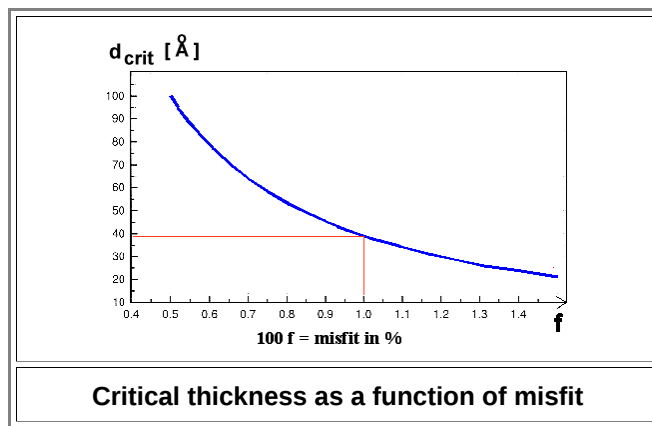
There is a dislocation after about 7 unit cells, which is a rather high density. In this case an [edge-on](#) HRTEM picture is sensible, because you would not be able to see anything "from the top". The dislocations are too closely spaced to detect them in any other way.

■ But now let's give the critical thickness d_A a closer look. It is not too difficult to calculate this quantity. The misfit, i.e. the difference in lattice constants, is of importance, of course, as are the elastic properties of the two materials, i.e. their Young's modulus. In the end a rather simple and approximate but good equation results that is shown graphically below.

And this equation is really, really bad news:

**The critical thickness is very small,
even for small misfit**

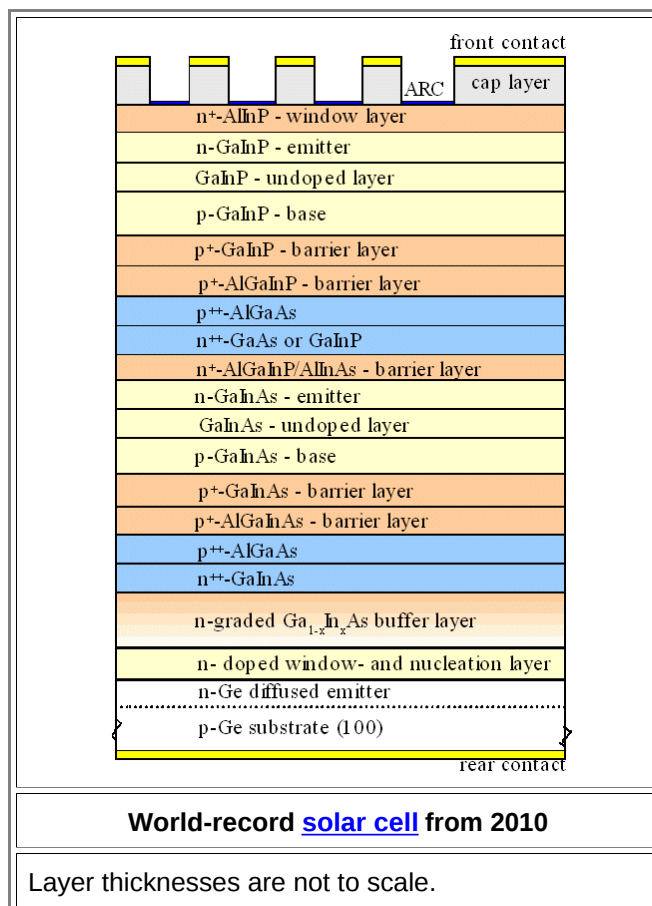
● Here is the "master" curve for preventing a lot of good semiconductor products:



For a misfit of just 1 %, the critical layer thickness is only about 40 Å or 4 nm! That is not much. We know a few tricks to enlarge the critical thickness somewhat, but you can't really beat it.

- Why is that bad news? Because it means that you cannot make layered structures of various semiconductors without producing misfit dislocations in the interphases for most cases. And if that happens, your device is electronically dead. It's that simple.

Why would we want make stacks of semiconductors? Because that's what we must do - otherwise a lot of important devices (like DVD players) would not exist. Let me give you just one example:



- We need to put a hell of a lot of different semiconductors on top of each other to make a very good solar cell. Same thing for Lasers, LED's, you name it. And most combinations of what we would like to do won't work because misfit dislocations cannot be avoided!

While the picture above might insinuate that there are plenty of possibilities left, it is not so. The semiconductors above have been every carefully chosen to do what is wanted of them as well as possible, while not generating misfit dislocations in the the various interphases. There is a lot of compromising and long hard work in this structure.

Making much better and simpler solar cells would be possible (and much easier) if we wouldn't have the misfit dislocation problem. Same thing for Lasers and so on, and for all those gadgets that don't even exist because of that problem

One last word. Thanks to oxygen, the atoms on both side of touching materials do *not* like to bond. If they would, the interphase formed when you and your partners skin touch, would not come apart again. Whatever you put on the table would be stuck there. You can easily come up with the plot for a nice horror movie, assuming that some evil aliens switched off the "do no bond across most interfaces" law.

Why is that? Because most surfaces already have formed an interface to their oxides. When you put a silicon wafer on top of another one, they will not easily bond because it is actually a thin layer of silicon (di)oxide (SiO_2) touching another thin layer of SiO_2 in just some places (surfaces are usually not atomically flat). And all the atoms are thus already quite happy with the (oxygen) partners they have and will not engage in a little fooling around.

For about the same reason your "skin-oxide" does not bond to that of your partner and you don't have to worry about misfit dislocations in the skin-skin interphase (about other misfits I don't know).

Fluorine (F) is even better than oxygen to satisfy bonding demands, and that's why nothing sticks to Teflon.