

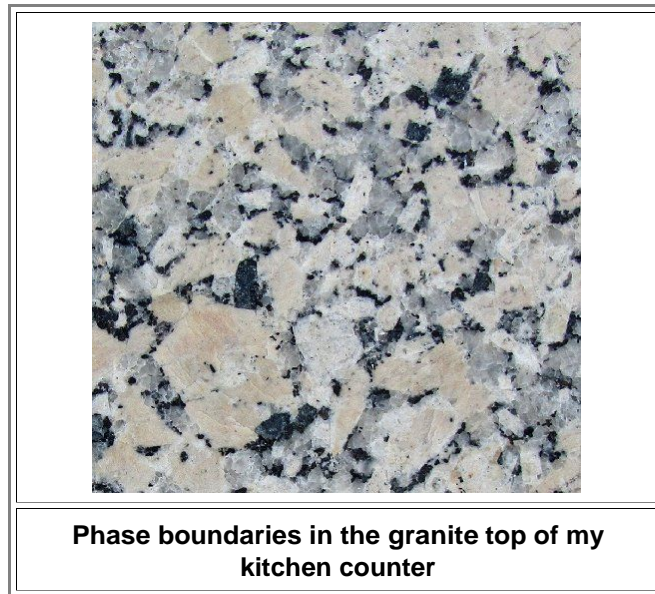
### 5.3.2 Phase Boundaries

Now let's look at **phase boundaries**, the second important two-dimensional defect.

- Like a grain boundary it has two sides but now different things (or, as we call it, different *phases*) are separated by a phase boundary. After all, our iron comes in more than one phase and on occasion we have both phases *simultaneously*.

Between two atomically connected phases we then must have a phase boundary by definition.

You have seen a lot of phase boundaries. Or maybe you didn't. There are none so blind as those who will not see. Fine, let me help you. In the following picture you can see a lot of phases and therefore also phase boundaries between the phases:

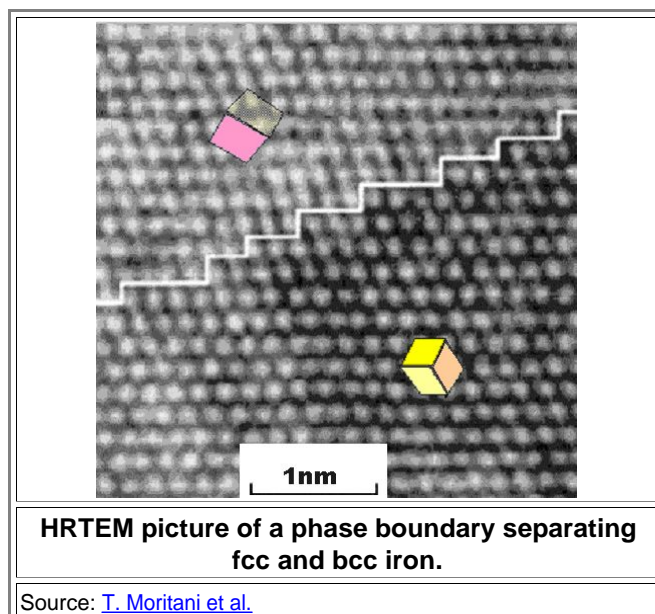


- Granite is always a mixture of quartz ( $\text{SiO}_2$ ) and some **feldspar** (silicates like  $\text{KAlSi}_3\text{O}_8$ ,  $\text{NaAlSi}_3\text{O}_8$ ,  $\text{CaAl}_2\text{Si}_2\text{O}_8$ , and many more) and, in this particular granite, some **mica** (the black stuff; rather complex sheet silicates, e.g.  $\text{KAl}_2[\text{AlSi}_3\text{O}_{10}(\text{OH})_2]$  or muscovite). So we have at least three phases mixed rather haphazardly.

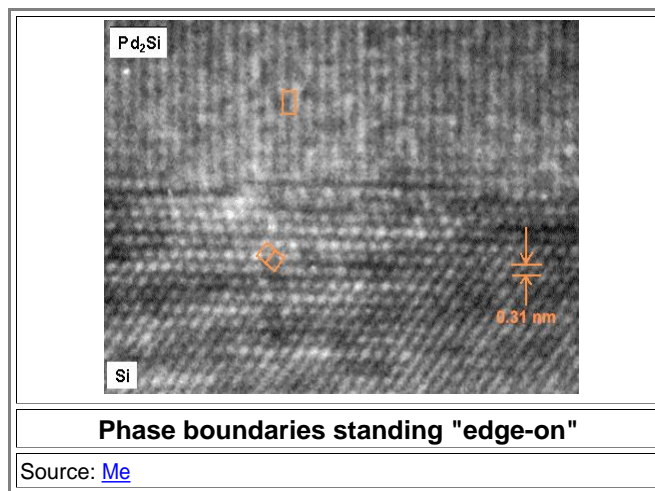
The boundary between the melt and a growing (or melting) crystal also constitutes a phase boundary, so you have seen phase boundaries whenever you have an ice cube in your whisky.

Your skin (loosely speaking) is a phase boundary. On one side is air, on the other side is you (in the form of bones and some slimy stuff).

More to the point, the boundary between a crystal of type A (for example pure bcc iron) and a crystal of type B (for example an iron carbide particle) is a phase boundary and so is the boundary between bcc iron and fcc iron that is shown below:



- The white line shows the position of the phase boundary and the insets show schematically the orientation of the cubic elementary cells. The white dots are columns of iron atoms.



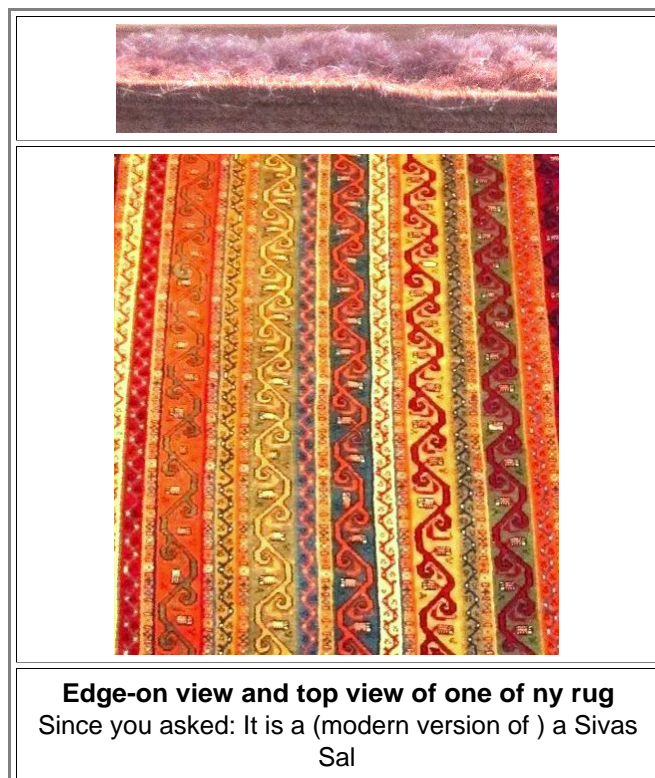
● This HRTEM picture shows a phase boundary between fcc silicon (Si) and hexagonal palladium silicide (Pd<sub>2</sub>Si). The white dots, just about recognizable, are columns of atoms once more.

▸ I admit that the phase boundary between fcc silicon (Si) and hexagonal palladium silicide (Pd<sub>2</sub>Si) might appear a bit out of phase here. **Silicides** from one of those material classes that you have never encountered before and are not important for swords. Nevertheless, they are quite important, e.g. for micro electronics.

● Chances are that you, personally, are also a direct user of a silicide without knowing that (hint: look for "molybdenum silicide" in the Net).

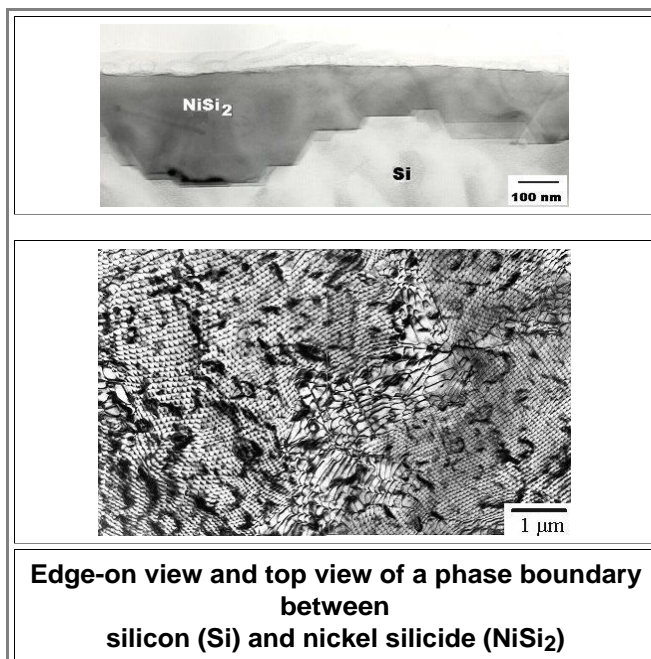
Be that as it may, I just happen to like the Pd<sub>2</sub>Si picture a lot. First, because to the best of my knowledge, it is the **very first** high-resolution TEM picture of a phase boundary ever taken, second, because it was taken by me in 1980.

▸ So, now you have seen two pictures of actual phase boundaries at atomic resolution. Or have you? Looking at two-dimensional things **only** edge-on is a bit deceiving. Here is an example that needs no further comment:



● You are going to miss something for sure, if you look at planar defects only edge-on!

▸ So let's look at some phase boundary in both views, too. I take some of my own pictures since I don't have to worry about copyright problems then.



- Wow! In the bottom picture a dense network of [misfit dislocations](#) is present. There certainly is a lot to see in the **top view** that you don't see *edge-on!* What you see is even more complicated than in the case of the [grain boundary structure](#), and you really don't want to know about this. You do? Good. Maybe you have a feeling that the detailed structure of phase boundaries could be important? Boy are you right! Pretty much *all* of semiconductor technology and in particular **optoelectronics** relies on **phase boundary engineering**. Turn to this [advanced module](#) *after* you have finished chapter 5.
  - What the picture also shows in a visual if qualitative way is that phase boundaries are high-energy defects, just like grain boundaries. We [just learned this](#) but it is good to repeat it. It should be clear by now that the crystal doesn't want phase boundaries [any more](#) than it wants grain boundaries. However, while it could get rid of grain boundaries in principle if not in practice, it *cannot* get rid of phase boundaries as long as it wants to have *precipitates* (meaning a completely enclosed second phase; [look a chapter ahead](#) if you don't know what that means) for nirvana reasons. In certain conditions the crystal *needs* to have precipitates for achieving nirvana; we will learn about that presently. The crystal now faces the classical problem that you can't have your cake *and* eat it. It can't have precipitates without having phase boundaries that envelop the precipitates. All it can do is to optimize the situation and that calls for having just a few large precipitates. All *we* can do in metal technology is to interfere with the this optimization process and coerce the crystal to do it in a way we like. Large precipitates result by the growth of originally small ones. What that means is that the phase boundary must *move*—just like grain boundaries when the grains grow.
- Now back to the topic. You guessed it: in sword making we need to move phase boundaries around quite a lot too, so we answer the standard question right away:

**Phase boundaries move as soon as atoms can move around**

- We have another phenomenon that depends on some *diffusion* process.
- ▶ The best examples for phase boundaries coming with precipitates are the iron carbide (Fe<sub>3</sub>C) particles invariably found inside steel. Whenever they grow or shrink, the phase boundary separating their surface from the crystal must move. And for doing this, *carbon atoms* must move, too.
- I'm not talking "theory" here but, for example, the making of **wootz steel blades** where the smith must grow the iron carbide particles to a rather large size.
- ▶ So just accept it. We will encounter phase boundaries a lot when we attempt to make any sword blade, and they will come up right again in the next paragraph.

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1) T. Moritani, N. Miyajima, T. Furuhashi, T. Maki: "Comparison of interphase boundary structure between bainite and martensite in steel" Scripta Materialia 47 (2002) p. 193–199  
 2) FÖLL, H., HO, P., TU, K.N.: "Cross-sectional TEM of silicon-silicide interfaces" J. Appl. Phys. 52 (1981) o. 25