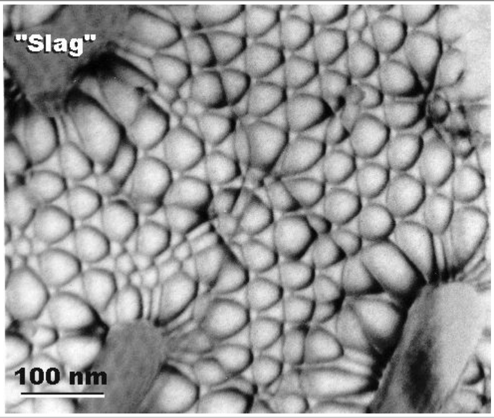
Pictures of Grain Boundaries

Old Pictures Taken be Me

- Here are a few transmission electron microscope (TEM) pictures of grain boundaries in silicon (Si) that I took around 1980. The HRTEM pictures were among the very first pictures ever taken at high resolution. Looking at grain boundaries edge-on you won't see much, so the first examples are "top-down".

  - You are looking right on the grain boundary. The silicon above and below the boundary is pretty much invisible. It's like looking at an old-fashioned slide. The glass plates on top and bottom of the film containing the picture are invisible.
    These grain boundaries were artificially *made* (by me) by "welding" two single crystals of silicon with a certain misalignment. This needs high temperatures and pressure, and is not unlike the "hammer welding" of two pieces of steel. In either case you produce a grain boundary with some inclusions from the "dirt" still present on the surface of the two pieces to be joined. In the case of silicon, the "dirt" would be silicon dioxide (SiO_2), in the case of iron, we call it iron oxide, scale or slag.

Illustration



Grain boundary in Si made by welding.

It's low-angle twist boundary on a {111} plane, if you must know.

  - There is a lot of structure on a rather small scale. The lines forming a kind of six-fold pattern are "**grain boundary dislocations**" with two kinds of embedded **stacking faults**. You really don't want to know more about this.
    The smooth blobs (one is marked "slag") are amorphous silicon dioxide (SiO_2) particles left over from the welding process—just like real slag particles are always found in hammer welded blades. Amorphous silicon dioxide, by the way, is just quartz glass; if it would be crystalline we call it rock crystal.

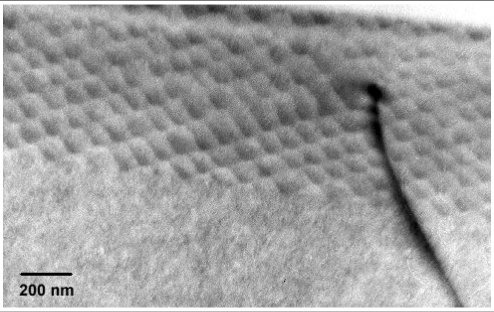
- Here is a picture of a very similar grain boundary:

Grain boundary in Si made by welding

Low angle twist boundary on {100}, if you must know.

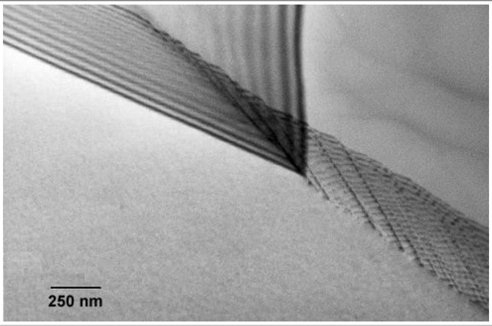
  - Same thing once more. Grain boundary dislocations forming a very regular pattern; hardly any "slag".

Here are two pictures of naturally occurring grain boundaries. They are all inclined to the viewing direction.



Large-angle grain boundary in silicon.

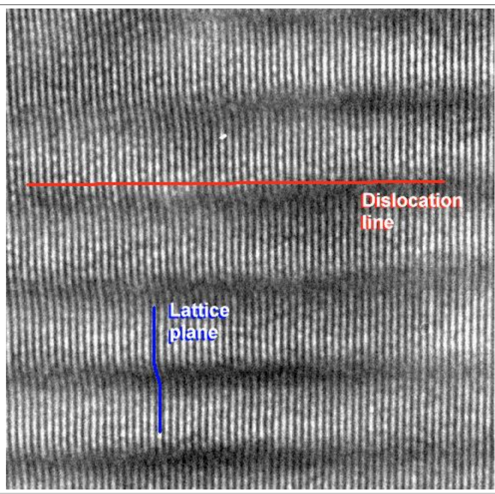
- The "chicken wire" structure indicates a network of very special grain boundary dislocations. The big black line is a "real" dislocation, running through one of the grains and ending at the grain boundary, interacting with the dislocations there.



Grain boundary junction in Si

- A junction of three large-angle grain boundaries. The lower one has clearly visible grain boundary dislocations With the eye of faith one also sees a fine-mashed network in the one branching off to the left. The one going up appears to without a structure (the "zebra" fringes have nothing to do with structures in the boundary) but that might simply be due to the limitations of the electron microscope.

Just for the hell of it, here are high–resolution transmission electron microscope (HRTEM) pictures at atomic resolution. Those pictures are among the very first ones taken with atomic resolution around 1979, when electron microscopes became powerful enough for that.

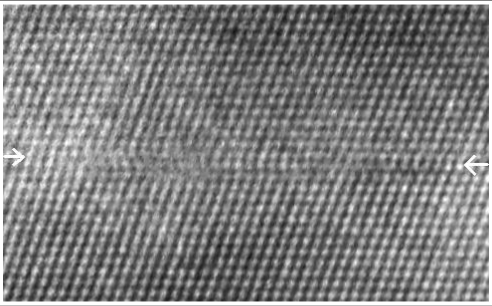


HRTEM picture of the grain boundary above.

Visible are 5 screw dislocations, causing the typical shift of the lattice planes.

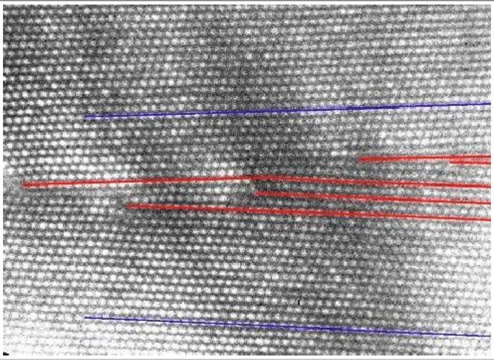
- What you see are "screw dislocations". Look up the "dislocation science" module if you feel you need to know what "screw dislocations" are. Otherwise screw them.

Here, just for the hell of it, is an "edge-on" picture at atomic resolution of the ("small-angle twist") grain boundary in the top most picture. There is really not much to see.



HRTEM picture of the grain boundary above .

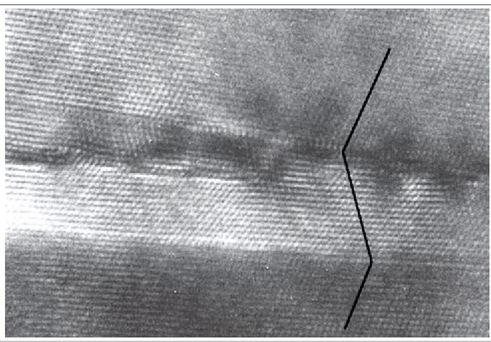
- Things get a bit better with "edge-on" pictures at atomic resolution of some slightly different kind of grain boundary ("small-angle tilt").



HRTEM picture of a small-angle tilt grain boundary.

- The boundary runs from left to right in the middle of the picture. The colored lines are only to guide the eye. The blue lines indicate that the orientation of the crystal above or below the boundary differs indeed by a "small angle".
  The red lines indicate ending lattice planes, i.e. edge dislocations.
  The picture shows directly (and for the first time) that this kind of boundary consists indeed of a lot of dislocations in some special array. This was predicted long before it could be imaged. Now the prediction has been proved.

The next picture shows some unusual and unexpected behavior that could only be found with "edge-on HRTEM". A simple (low-angle tilt) boundary is actually not so simple but consists of three boundaries close together.



HRTEM picture of complex boundary consisting of three boundaries. .

- A low-angle tilt boundary composed of individual dislocations as in the picture above is actually sandwiched between two so-called "twin" boundaries, the effects of which cancel each other. That is shown by the black lines that bend substantially at the twin boundaries, but in opposite directions.
  The misorientation between the upper part and the lower part of the crystal is only determined by the low-angle tilt boundary. It changes position from in-between the twin boundaries to being superimposed on one of the twins.

- This effect would be easily missed looking at the grain boundary "top-down", so edge-on views do have some merits

So what are you supposed to learn form all this stuff? Not much, really. The messages are simple:

- The internal structure of grain boundaries is very complex. Trying to understand in detail what one sees on those pictures will take a lot of time and effort.
- Nevertheless, it is great fun (not to mention a lot of work) to take pictures like the ones above.