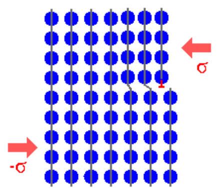
5. Dislocations

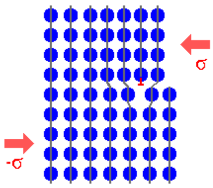
5.1 Basics

5.1.1 Burgers and Line Vector

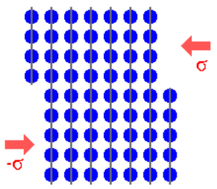
- The ***smelting*** and ***forging*** of metals marks the beginning of civilization - the *art* of working metals was for thousands of years the major "high tech" industry of our ancestors.
  - Trial and error over this period of time lead to an astonishing degree of perfection, as can be seen all around us and in many museums. In the state museum of **Schleswig-Holstein** in **Schleswig**, you may admire the **damascene blades** of our **Viking** ancestors.
  - Two kinds of iron or steel were welded together and forged into a sword in an extremely complicated way; the process took several weeks of an expert smith's time. All this toil was necessary if you wanted a sword with better properties than those of the ingredients. The damascene technology, shrouded in mystery, was needed because the vikings didn't know a thing about defects in crystals - exactly like the Romans, Greek, Japanese (india) Indians, and everbody else in those times.
  - You might enjoy finding and browsing through several modules to this topic which are provided "on the side" in this Hyperscript.
- Exactly *why* metals could be plastically deformed, and *why* the plastic deformation properties could be changed to a very large degree by forging (and magic?) without changing the chemical composition, was a mystery for thousands of years.
  - No explanation was offered before **1934**, when **Taylor**, **Orowan** and **Polyani** discovered (or invented?) independently the **dislocation**.
  - A few years before (**1929**), U. **Dehlinger** (who, around **1969** tried to teach me basic mechanics) almost got there, he postulated so-called "*Verhakungen*" as lattice defects which were supposed to mediate plastic deformation - and they were almost, but not quite, the real thing.
- It is a shame up to the present day that the discovery of the basic scientific principles governing metallurgy, still the most important technology of mankind, did not merit a **Nobel prize** - but after the war everything that happened in science before or during the war was eclipsed by the atomic bomb and the euphoria of a radiantly beautiful nuclear future. The link pays tribute to some of the men who were instrumental in solving one of the oldest scientific puzzles of mankind.
- Dislocations can be perceived easily in some (mostly two-dimensional) structural pictures on an atomic scale. They are usually introduced and thought of as extra lattice planes inserted in the crystal that do not extend through all of the crystal, but end in the dislocation line.
  - This is shown in the schematic **three-dimensional view** of an edge dislocations in a cubic primitive lattice. This beautiful picture (from Read?) shows the inserted half-plane very clearly; it serves as the quintessential illustration of what an *edge* dislocation looks like.
- Look at the picture and try to grasp the concept. *But don't forget*
  - **1.** There is *no such crystal* in nature: All real lattices are more complicated - either not cubic primitive or with more than one atom in the base.
  - **2.** The *exact structure* of the dislocation will be more complicated. *Edge* dislocations are just an extreme form of the possible dislocation structures, and in most real crystals would be split into "partial" dislocations and look much more complicated.
- We therefore must introduce a more general and necessarily more abstract definition of what constitutes a dislocation. Before we do that, however, we will continue to look at some properties of (edge) dislocations in the simplified atomistic view, so we can appreciate some elementary properties.
  - *First*, we look at a simplified but principally correct rendering of the connection between **dislocation movement** and **plastic deformation** - the elementary process of metal working which contains all the ingredients for a complete solution of all the riddles and magic of the smith's art.



Generation of an edge dislocation by a *shear* stress



Movement of the dislocation through the crystal



Shift of the upper half of the crystal after the dislocation emerged

- This sequence can be seen **animated** in the link

This calls for a little exercise

Exercise 5.1-1

Find the mistakes

What the picture illustrates is a simple, but far-reaching truth:

Plastic deformation proceeds - atomic step by atomic step - by the

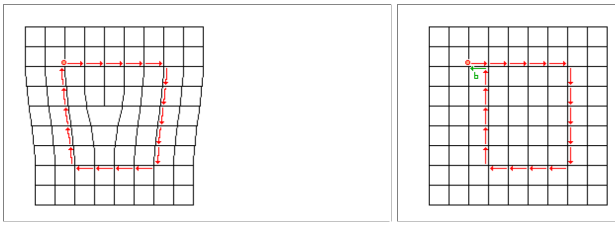
generation and movement of dislocations

- The whole art of forging consists simply of manipulating the *density* of dislocations, and, more important, their *ability of moving* through the lattice.
- After a dislocation has passed through a crystal *and* left it, the lattice is complely restored, and no traces of the dislocation is left in the lattice. Parts of the crystal are now shifted in the plane of the movement of the dislocation (left picture). This has an interesting consquence: *Without dislocations, there can be no elastic stresses whatsoever in a single crystal!* (discarding the small and very localized stress fields around point defects).

We already know enough by now, to deduce some elementary properties of dislocations *which must be generally valid*.

- **1.** A dislocation is **one-dimensional defect** because the lattice is *only* disturbed along the **dislocation line** (apart from small elastic deformations which we do not count as defects farther away from the core). The dislocation line thus can be described at any point by a **line vector** ***t(x,y,z)***.
- **2.** In the **dislocation core** the bonds between atoms are *not* in an equilibrium configuration, i.e. at their minimum enthalpy value; they are heavily distorted. The dislocation thus must possess *energy* (per unit of length) and *entropy*.
- **3.** Dislocations *move* under the influence of external forces which cause internal stress in a crystal. The area swept by the movement defines a plane, the **glide plane**, which always (by definition) contains the dislocation line vector.
- **4.** The movement of a dislocation *moves the whole crystal* on one side of the glide plane relative to the other side.
- **5.** (Edge) dislocations could (in principle) be generated by the *agglomeration of point defects*: self-interstitial on the extra half-plane, or vacancies on the missing half-plane.

Now we add a new property. The fundamental quantity defining an arbitrary dislocation is its **Burgers vector *b***. Its atomistic definition follows from a **Burgers circuit** around the dislocation in the real crystal, which is illustrated below



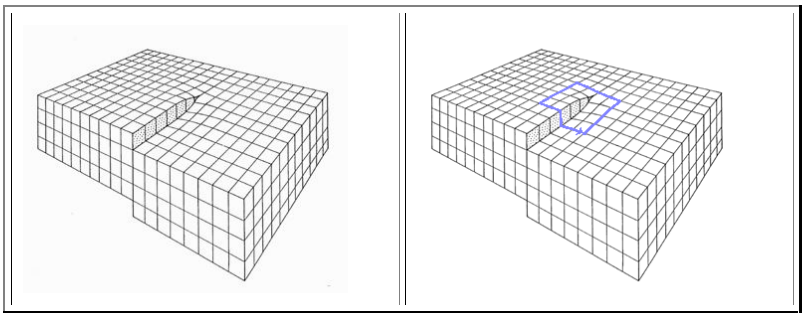
- *Left picture*: Make a closed circuit that encloses the dislocation from lattice point to lattice point (later from atom to atom). You obtain a closed chain of the base vectors which define the lattice.
- *Right picture*: Make exactly the same chain of base vectors in a perfect reference lattice. *It will not close*.

- The special vector needed for closing the circuit in the reference crystal is *by definition* the *Burgers vector* ***b***.

- It follows that the *Burgers vector* of a (perfect) dislocation is of necessity a *lattice vector*. (We will see later that there are exceptions, hence the qualifier "perfect").

- *But beware!* As always with conventions, you may pick the *sign* of the Burgers vector at will.
  - In the version given here (which is the usual definition), the closed circuit is around the dislocation, the Burgers vector then appears in the reference crystal.
  - You could, of course, use a closed circuit in the reference crystal and define the Burgers vector around the dislocation. You also have to define if you go clock-wise or counter clock-wise around your circle. You will always get the same vector, but the sign will be different! And the sign is very important for calculations! So whatever you do, *stay consistent!*. In the picture above we went clock-wise in both cases.

- Now we go on and learn a new thing: There is a second *basic* type of dislocation, called **screw dislocation**. Its atomistic representation is somewhat more difficult to draw - but a Burgers circuit is still possible:



  - You notice that here we chose to go *clock-wise* **-** for no particularly good reason

- If you imagine a walk along the non-closed Burges circuit, which you keep continuing round and round, it becomes obvious how a **screw dislocation** got its name.
  - It also should be clear by now how Burgers circuits are done.
  - But now we will turn to a more formal description of dislocations that will include *all possible cases*, not just the extreme cases of pure edge or screw dislocations.

Exercise 5.1-3
Quick Questions to 5.1