5.2.3 Energy of a Dislocation

- With the results of the elasticity theory we can get approximate formulas for the **line energy** of a dislocation and the elastic interaction with other defects, i.e. the forces acting on dislocations.
  - The energy of a dislocation comes from the elastic part that is contained in the elastically strained bonds outside the radius r_0 *and* from the energy stored in the core, which is of course energy sitting in the distorted bonds, too, but is not amenable to elasticity theory.
  - The *total* energy per unit length E_{ul} is the sum of the energy contained in the elastic field, E_{el}, and the energy in the core, E_{core} .

$$E_{ul} = E_{el} + E_{core}$$

  - *Do not confuse energies **E** with Youngs modulus **Y** which is often (possibly here) written as **E**, too! From the context it is always clear what is meant.*
  - Using the formula for the strain energy for a volume element given before, integration over the total volume will give the total elastic energy E_{el} of the dislocation. The integration is easily done for the screw dislocation; in what follows the equations are always *normalized to a unit of length*.

$$dE_{el}(\text{screw}) = \pi \cdot r \cdot dr \cdot (\sigma_{\Theta z} \cdot \epsilon_{\Theta z} + \sigma_{z\Theta} \cdot \epsilon_{z\Theta}) = 4\pi \cdot r \cdot dr \cdot G \cdot (\epsilon_{\Theta z})^2$$

$$E_{el}(\text{screw}) = \frac{G \cdot b^2}{4\pi} \cdot \int_{r_0}^{R} \frac{dr}{r} = \frac{G \cdot b^2}{4\pi} \cdot \ln \frac{R}{r_0}$$

  - The integration runs from r_0, the core radius of the dislocation to R, which is some *as yet undetermined* external radius of the elastic cylinder containing the dislocation. In principle, R should go to infinity, but this is not sensible as we are going to see.
- The integration for the edge dislocation is much more difficult to do, but the result is rather simple, too:

$$E_{el}(\text{edge}) = \frac{G \cdot b^2}{4\pi(1 - \nu)} \cdot \ln \frac{R}{r_0}$$

  - So, apart from the factor $(1 - \nu)$, this is the same result as for the screw dislocation.
- Let us examine these equations. There are a number of interesting properties; moreover, we will see that there are very simple approximations to be gained:
- **1.** *The total energy **U** of a dislocation is proportional to its length **L**.*

$$U = E_{ul} \cdot L = L \cdot (E_{el} + E_{core})$$

  - Since we always have the principle of minimal energy (entropy does not play a role in this case), we can draw a important conclusion:
  - *A dislocation tends to be straight* between its two "end points" (usually dislocation knots). That is a *first* rule about the direction a dislocation likes to assume.
- **2.** *The line energy of an edge dislocation is always larger than that of a screw dislocation* since $(1 - \nu) < 1$. With $\nu \approx 1/3$, we have $E_{screw} \approx 0{,}66 \cdot E_{edge}$.
  - This means that a dislocation tends to have as large a screw component as possible. This is a *second* rule about the direction a dislocation likes to assume *which may be in contradiction* to the first one. It is quite possible that a dislocations needs to zig-zag to have as much screw character as geometrially allowed - it then cannot be straight at the same time.
- **3.** *The elastic part of the energy depends (logarithmically) on the crystal size* (expressed in R), *for an infinite crystal it is infinite (∞)!* Does this make any sense?
  - Of course this doesn't make sense. Infinite crystals, however, do not make sense either. And in finite crystals, even in *big* finite crystals, the energy is finite!

- Moreover, in most real crystals it is *not* the outer dimension that counts, but the size of the grains which are usually quite small. In addition, if there are many dislocations with different signs of the Burgers vector, their strain fields will (on average) tend to cancel each other. So for *practical* cases we have a finite energy.

4. *The elastic part of the energy also depends (logarithmically) on the core radius* r_0.

5. *The energy is a weak function of the crystal (or grain size)* R.

- Taking an extremely small value for r_0, e.g. **0,1 nm**, we obtain for **ln** (R/r_0) an extreme range of **20,7 - 2,3** if we pick extreme values for R of **100 mm** or **1 nm**, respectively. A more realistic range for R would be **100 µm - 10 nm**, giving **ln** (R/r_0) **= 13,8 - 4,6**. Grain size variations, within reasonable limits, thus only provide a factor of **2 - 3** for energy variations.

We will now deduce an approximation for the line energy that is sufficiently good for most purposes.

- We equate r_0 with the magnitude of the Burgers vector, $|\underline{b}|$. This makes sense because the Burgers vector is a direct measure of the "strength" of a dislocation, i.e. the strength of the displacement in the core region.
- We need a value for the energy in the core of the dislocations, which so far we have not dealt with. Since there is no easy way of calculating that energy, we could equate it in a first approximation with the energy of melting. That would make sense because the dislocation core is comparable in its degree of distortion to the liquid state. More sophisticated approaches end up with the best **simple** value:

$$E_{core} = \frac{G \cdot b^2}{2\pi}$$

- There are, however, other approaches, too.
- The total energy for $r_0 = b$ then becomes

$$E_{tot} = \frac{G \cdot b^2}{4\pi} \cdot \left(\ln \frac{R}{b} + 2 \right)$$

More generally, the following formula is often used

$$E_{tot} = \frac{G \cdot b^2}{4\pi(1 - \nu)} \cdot \left(\ln \frac{R}{b} + B \right)$$

- with B = pure number best approximating the core energy of the particular case. Often $B = 1$ is chosen, leading to

$$E_{tot} = \frac{G \cdot b^2}{4\pi(1 - \nu)} \cdot \left(\ln \frac{R}{b} + 1 \right) = \frac{G \cdot b^2}{4\pi(1 - \nu)} \cdot \left(\ln \frac{e \cdot R}{b} \right)$$

- For the last equation bear in mind that **ln(e) = 1**.

The **ln** term is not very important. To give an example; it is exactly **4π** for $\mathbf{e \cdot R = 3{,}88 \times 10^4\,|b|}$, i.e. for $R \approx$ **5 µm** ; the total energy in this case would be $E_{tot} = 2G \cdot b^2$.

- In a very general way we can write

$$E_{tot} = \alpha \cdot G \cdot b^2$$

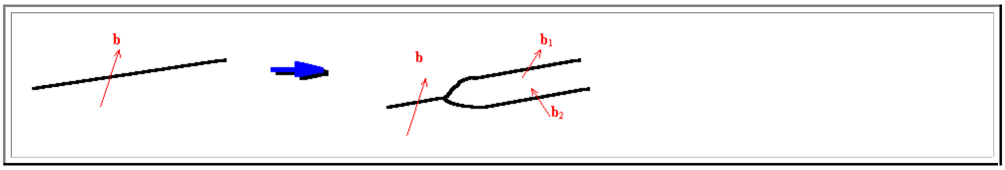
- And α (from measurements) is found to be α ≈ **1,5 ....0,5**. If we do not care for factors in the order of unity, we get the final *very simple formula* for the **line energy** of a dislocation

$$E_{total} \approx G \cdot b^2$$

- With this expression for the line energy of a dislocation, we can deduce more properties of dislocations.
- **6.** *Dislocations always tend to have the smallest possible Burgers vector*.
  - Since for Burgers vectors $\underline{\boldsymbol{b}}_i$ larger than the smallest translation vector of the lattice and thus expressible by $\underline{\boldsymbol{b}}_i = \underline{\boldsymbol{b}}_1 + \underline{\boldsymbol{b}}_2$; $\underline{\boldsymbol{b}}_{1,2}$ = some shorter vectors of the lattice, we always have

$$(b_1)^2 + (b_2)^2 < b^2$$

  - A splitting into smaller Burgers vectors is therefore always energetically favorable.
- There are therefore no dislocations with large Burgers vectors!
  - If a dislocation would have a large Burgers vector, it would immediately split into two (or more) dislocations with smaller Burgers vectors.
  - This is *always* possible, because in the Volterra construction you can always replace *one* cut with the translation vector $\underline{\boldsymbol{b}}$ by *two* cuts with $\underline{\boldsymbol{b}}_1$ and $\underline{\boldsymbol{b}}_2$ so that $\underline{\boldsymbol{b}} = \underline{\boldsymbol{b}}_1 + \underline{\boldsymbol{b}}_2$.



- **7.** *The line energy is in the order of **5 eV** per Burgers vector.*.
  - This makes dislocations automatically non-equilibrium defects. They will not come into being out of nothing like point defects for free enthalpy reasons.
- **8.** *The line energy (= energy per length) has the same dimension as a a force*, it expresses a **line tension** , i.e. a force in the direction of the line vector which tries to shorten the dislocation.
  - It actually *is* a force, as we can see from the definition of such a line tension $\boldsymbol{F}$:

$$F = -\frac{dU}{dL}$$

  - We thus may imagine a dislocation as a stretched rubber band, which tries to be as short as possible. But one should be careful not to overreach this analogy. Ask yourself: What keeps dislocations loops stable?