2.4.4 Schwingungsfrequenz der Atome in Kristallen

Note: Youngs Modulus (= Elastizitätsmodul) is abbreviated with an "***E***" in this text; not with a "***Y***" as is customary in the English literature.

We have already employed the picture of an atom or particle oscillating (or vibrating) in its potential well. Now we shall compute the vibration frequency $\omega = 2\pi\nu$ from the binding potential.

- As long as the potential increases quadratically with the distance from the equilibrium position r_0, the restoring force will be proportional to the deviation $x = r - r_0$ from r_0; and we have a simple harmonic oscillator.
- The *harmonic* approximation is good enough for getting an order of magnitude estimate of the vibration frequency; i.e. we simply replace the proper potential by its Taylor expansion around r_0 and stop after the quadratic term. We already did that; we had

$$U = U_0 + 1/2U_0'' \cdot x^2$$

and

$$U''(r_0) = U_0 \cdot (nm/r_0^2)$$

The basic equation for oscillations in this potential that we have to solve is

$$m_a \cdot \frac{d^2x}{dt^2} + k_s \cdot x = 0$$

- with m_a = mass of the vibrating particle (we use the symbol m_a instead of m to avoid confusion with the exponent m in the potential equation). In this formulation we also used a "**spring constant**" k_s in order to be able to compare the solutions with standard formulations of classical mechanics.
- The resonance frequency ω of the system is known from standard mechanics; it is

$$\omega = \left(\frac{k_s}{m_a}\right)^{1/2}$$

- (Try it; all you have to do is to see of the solution $x = x_0 \cos \omega t$ is a solution for the differential equation above).
- While for a real oscillator there will always be some friction (or better energy dispersion); i.e. a term $k_f \cdot dx/dt$, we do not have to worry about that because friction does not change the resonance frequency. If you want to know more about this, use the link.

We know the or restoring force F_{res} of our system, it is simply

$$F_{res} = -\frac{dU}{dx} = -U_0'' \cdot x = U_0 \cdot (nm/r_0^2) \cdot x$$

- The spring constant thus is simply $k_s = U_0 \cdot (nm/r_0^2)$, and the resonance frequency is

$$\omega = \left(\frac{U_0 \cdot (nm/r_0^2)}{m_a}\right)^{½} = \frac{1}{r_0}\left(\frac{U_0 \cdot n \cdot m}{m_a}\right)^{½}$$

While this is good enough, we remember that we had the second derivative of the potential at some other occasion: When we found a formula for Youngs modulus E.

- What we had was

$$E = \frac{1}{r_0} \cdot \frac{d^2U}{dr^2} = \frac{n \cdot m \cdot U_0}{r_0^3}$$

- It is easy enough to use ***E*** instead of the spring constant, we have

$$k_S = U_0 \cdot \frac{n \cdot m}{r_0^2} = E \cdot r_0$$

- Which gives

$$\omega = \left(\frac{E \cdot r_0}{m_a}\right)^{1/2}$$

The vibration frequency of an atom in a lattice thus will be determined - approximately - by the easily obtainable quantities Youngs modulus, lattice constant and mass of the atom. Lets see what we get for some examples

- Lets take Silicon. We have

$$E = 150\ \text{GPa} = 1{,}5 \cdot 10^{11}\ \text{N/m}^2$$

$$m_a = 31 \cdot 1{,}67 \cdot 10^{-27}\ \text{kg} \quad \Rightarrow \quad \omega = 8{,}4 \cdot 10^{13}\ \text{Hz}, \quad \nu = 1{,}34 \cdot 10^{13}\ \text{Hz}$$

$$r_0 = 0{,}31\ \text{nm} = 3{,}1 \cdot 10^{-10}\ \text{m}$$

That is very satisfactory because it gives us the common result, always just claimed without justification, that the vibration frequency of atoms in a lattice is in the order of **10^{13} Hz**.

- That the vibration frequency of atoms in a solid is in the order of $\nu \approx$ **10^{13} Hz** is a number we will commit to memory now, and which we will never forget!

Is a frequency of **10^{13} Hz** large or small? Dumb question, you always have to add "In relation to what"?

- In electrical engineering, the highest frequencies "commonly" employed are in the **(1 - 100) GHz = 10^9 Hz - 10^{11} Hz** "Microwave" range. However, there is a lot of excitement about novel devices in the "Terahertz" (**= THz = 10^{12} Hz**) region. Our atoms, however, vibrate still faster - but not much.
- What is the frequency of visible light? Easy. We know its energy ***E* = h**ν, and we *must* know that the energy of visible light is in the **1 eV** region. It's actually a bit higher, **1 eV** is still infrared, but it is good enough for our purpose. With **h = 4.13 · 10^{-15} eV·s** (look it up!), we get $\nu_{light} \approx$ **2 · 10^{14} Hz**. So our atoms are a bit slower, but **10^{13} Hz** is a rather large frequency, indeed.