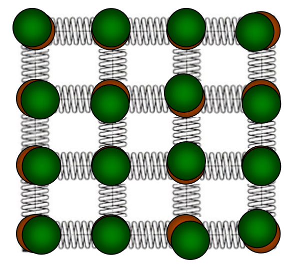
Chapter 4: continued
Atomic Vibrations

Every atom in a solid material is vibrating very rapidly about its lattice position within the crystal

- typical vibration frequency: 10^{13} Hz
- typical vibration amplitude: 10^{-3} nm = 10^{-12}m

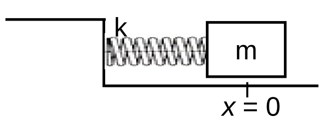


Atomic vibrations have many consequences:

- X-ray peaks are not sharp
- responsible for heat capacity and transport
- melting, when amplitude is high enough
- responsible for electrical resistance

Why frequencies are so high?

- Basically, because atoms are so light
- Consider the simple harmonic oscillator model



$$F(x) = m\frac{d^2x}{dt^2} = -kx$$

Potential energy of a spring:

$$U(x) = \frac{1}{2}k(x - x_o)^2$$

Frequency: $f = \frac{\omega}{2\Pi} = \frac{1}{2\Pi}\sqrt{\frac{k}{m}}$

Potential energy

$$U(x) = \frac{1}{2}k(x - x_o)^2$$

Almost any potential energy with the minimum can be approximated by a parabola (as long as we stay close enough to the minimum)

$$U(r) \approx U(r_o) + U'(r_o)(r - r_o) + \frac{1}{2}U''(r_o)(r - r_o)^2$$

Zero-point of PE irrelevant

parabola

Comparing to the PE of a spring, we identify $k = \left.\frac{\partial^2 U}{\partial r^2}\right|_{r0}$

Example: NaCl crystal

Model: $U(r) = -\frac{A}{r} + \frac{B}{r^8}$, where A = 1.31eV nm, B = 2.33×10^{-5}eV nm^8

Force constant k values: comparison

$$k \sim Y \times \boldsymbol{a}$$

a – lattice parameter, nm; *Y* – constant (Young's modulus)

Element	m, amu	Lattice parameter, *a*, nm	Frequency ω, rad s^{-1}	Force constant k, N m^{-1}
Diamond	12	0.154	8.54×10^{13}	146
Cu	64	0.256	1.77×10^{13}	33.3
Pb	207	0.350	3.90×10^{12}	5.25

- Atoms of **low** mass which are connected by **strong** bonds vibrate rapidly
- Atoms of **high** mass connected by **weak** bonds vibrate comparatively slowly

Amplitude of atomic vibrations

By treating the atoms as simple harmonic oscillators and assuming that the average thermal energy of an atom at temperature T is $k_B T$ → the amplitude of the atomic vibrations x_{max}

For any harmonic oscillator the potential energy at distance x from the equilibrium position is $0.5\,k\,x^2$, where k is the force constant. At the maximum amplitude, x_{max}, all of the energy of the oscillator is potential energy

$$E = \frac{p^2}{2m} + \frac{k(x-x_o)^2}{2} = kT + \frac{k(x-x_o)^2}{2} \text{(in 1D)}$$

$$\frac{1}{2}kx_{\max}^2 = k_B T$$

$$x_{\max} = \sqrt{\frac{2k_B T}{k}}$$

The energy of one atom moving along one direction (x) is written as (more next semester!):

Thermal vibrations of the atoms

Q.: Given that the actual value of *k* for Cu is about 100 N m^{-1} and the atomic spacing is 0.256nm, estimate the amplitude of vibration of the atoms at (a) 300K and (b) 1200K as a percentage of the equilibrium spacing.