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:

$$U(x) = \frac{1}{2} k(x - x_0)^2$$

Frequency:

$$f = \frac{\omega}{2\pi} = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$$
Potential energy

\[ U(x) = \frac{1}{2} k(x-x_0)^2 \]

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

Comparing to the PE of a spring, we identify \( k = \frac{\partial^2 U}{\partial r^2} |_{r_o} \)

Example: NaCl crystal

Model: \( U(r) = -\frac{A}{r} + \frac{B}{r^6} \), where \( A = 1.31\text{eV nm} \), \( B = 2.33 \times 10^{-5}\text{eV nm}^8 \)

Force constant \( k \) values: comparison

\[ k \sim Y \times a \]

\( a \) – lattice parameter, nm; \( Y \) – constant (Young’s modulus)

<table>
<thead>
<tr>
<th>Element</th>
<th>m, amu</th>
<th>Lattice parameter, ( a ), nm</th>
<th>Frequency ( \omega ), rad s(^{-1} )</th>
<th>Force constant ( k ), N m(^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diamond</td>
<td>12</td>
<td>0.154</td>
<td>8.54\times10^{13}</td>
<td>146</td>
</tr>
<tr>
<td>Cu</td>
<td>64</td>
<td>0.256</td>
<td>1.77\times10^{13}</td>
<td>33.3</td>
</tr>
<tr>
<td>Pb</td>
<td>207</td>
<td>0.350</td>
<td>3.90\times10^{12}</td>
<td>5.25</td>
</tr>
</tbody>
</table>

- 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 $k_B T \rightarrow$ the amplitude of the atomic vibrations $x_{\text{max}}$

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, $x_{\text{max}}$, all of the energy of the oscillator is potential energy

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

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

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

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

Chapter 4

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.