Physics with neutrons 1

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Exercise sheet 9
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Exercise 9.1

The Debye–Waller factor is used in to describe the attenuation of coherent neutron scattering caused by thermal motion:

$$f_{\mathrm{DWF}} = e^{-Q^2/3\langle u^2\rangle} = e^{-2W(\mathbf{Q})}.$$

For a cubic Bravais lattice we can make the following approximation:

$$2W = \frac{Q^2\hbar}{6MN}\int \frac{Z(\omega)}{\omega}\coth\left(\frac{\hbar\omega}{2k_BT}\right)d\omega,$$

where $Z(\omega)$ is the phonon density of states, M is the mass of the atom and N is the number of atoms in the crystal.
Within the Debye approximation, when the velocity of sound is frequency independent, we can express the phonon density of states for a cubic crystal with side length L by (in analogy with the theory of the black body radiation):

$$Z(\omega) = \frac{1}{2\pi^2}L^3\left(\frac{1}{c_L^3}+\frac{2}{c_T^3}\right)\omega^2. \tag{1}$$

c_L and c_T are the longitudinal and transverse velocity of sound, respectively. The total number of normal modes is $3N$. Therefore, we can put:

$$3N = \int_0^{\Omega_D} Z(\omega)d\omega. \tag{2}$$

ω_D is the maximum frequency of the normal mode and $\omega_D = \frac{\hbar\omega_D}{k_B}$ is the Debye temperature.

1. Calculate ω_D from the equations (1) and (2).
2. Calculate the asymptomatic behaviour of $2W$ for $T \ll \Theta_D$ and $T \gg \Theta_D$.
3. Copper crystallizes in fcc-lattice ($a = 3.615$ Å, $\rho_{\mathrm{Cu}} = 8920kg/m^3$, $c_L = 4760m/s$ and $c_T = 2320m/s$);
   a) Calculate θ_D and show that the obtained value is reasonable.
   b) Figure 1 and 2 show $Z(\omega)$ and the dispersion relation for copper, respectively (Nilsson 1973). What are the reasons of deviations to the Debye model?

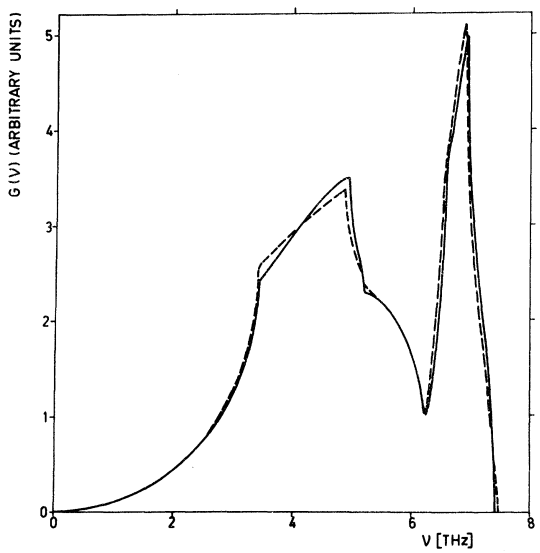

Figure 1: Phonon frequency distributions calculated from the Born-von Kármán models.

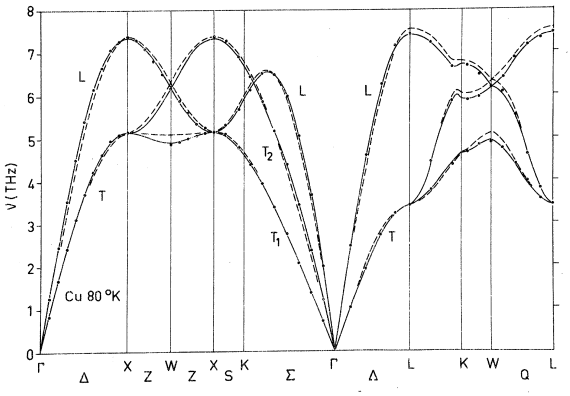

Figure 2: Dispersion curves for Cu at $80K$.

4. Calculate the mean amplitude $\langle u^2 \rangle$ for copper at $T = 20K, 100K, 500K, 1000K$.

5. Estimate the attenuation in a neutron powder diffraction measurement with wavelength $\lambda = 1.188$ Å of (100) and (440) reflex due to the Debye-Waller factor ($T = 200K$).

6. a) Why do soft materials have a larger Debye-Waller factor than condensed matter?
   b) What is the influence of mass on the Debye-Waller factor?

Happy Holidays!