Physics with Neutrons I

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Exercise sheet 5

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wiki.mlz-garching.de/n-lecture05:index

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

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

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

$$2W = \frac{Q^2\hbar}{6MN}\int \frac{Z(\omega)}{\omega}\coth\left(\frac{\hbar\omega}{2k_BT}\right)d\omega, \tag{1}$$

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):

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

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:

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

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

1. Find $Z(\omega)$ in terms of ω_D using the equations (2) and (3) and the definition $\dfrac{3}{c_s^3} = \dfrac{1}{c_L^3}+\dfrac{2}{c_T^3}$.
2. Calculate the asymptomatic behavior of $2W$ for $T \ll \theta_D$ and $T \gg \theta_D$.
3. Copper crystallizes in fcc-lattice (a = 3.615 Å, ρ_{Cu} = 8920 kg/m^3, c_L = 4760 m/s and c_T = 2320 m/s);
   (a) Calculate θ_D and show that the obtained value is reasonable.
   (b) Figures 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?

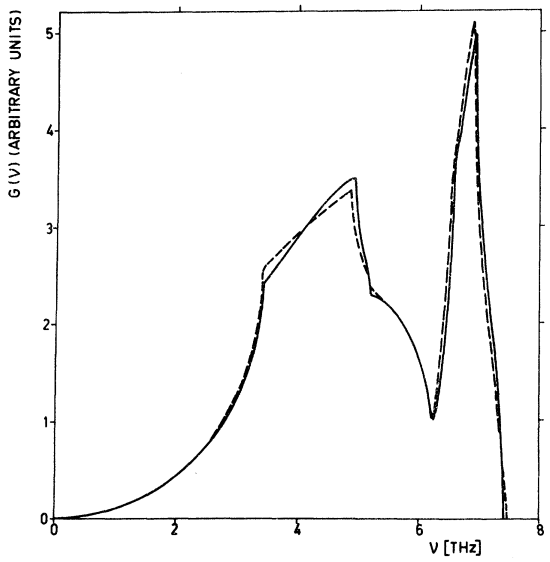

Figure 1: Phonon frequency distributions calculated from the Born-von Kármán models.

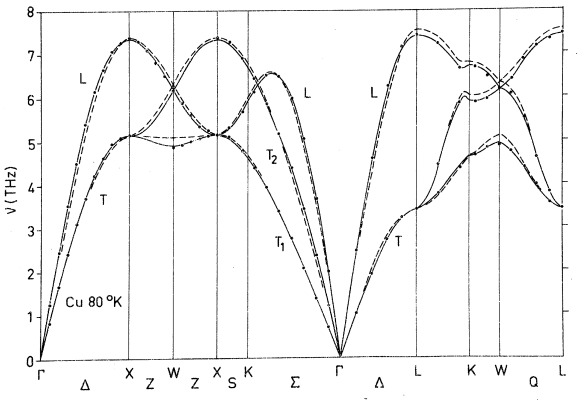

Figure 2: Dispersion curves for Cu at $80K$.

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

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

6. Why do soft materials (e.g. polymers, biological matter) have a larger Debye-Waller factor than hard materials (e.g. metals)?

   What is the influence of mass on the Debye-Waller factor?

Happy non-denominational winter solstice period!