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Problem sheet 7: Brillouin zone, Phonons, Heat capacity **29.11.2023**

7.1. Phonon spectrum (7 P)

Consider the phonon spectrum shown in the figure. It belongs to an fcc crystal with the lattice parameter $a = 5.64$ Å. You can read the exact phonon frequencies ($\nu = \omega/(2\pi)$) by zooming into the figure or by exploring this spectrum at the Materials Project (use the "Interactive plots" link).

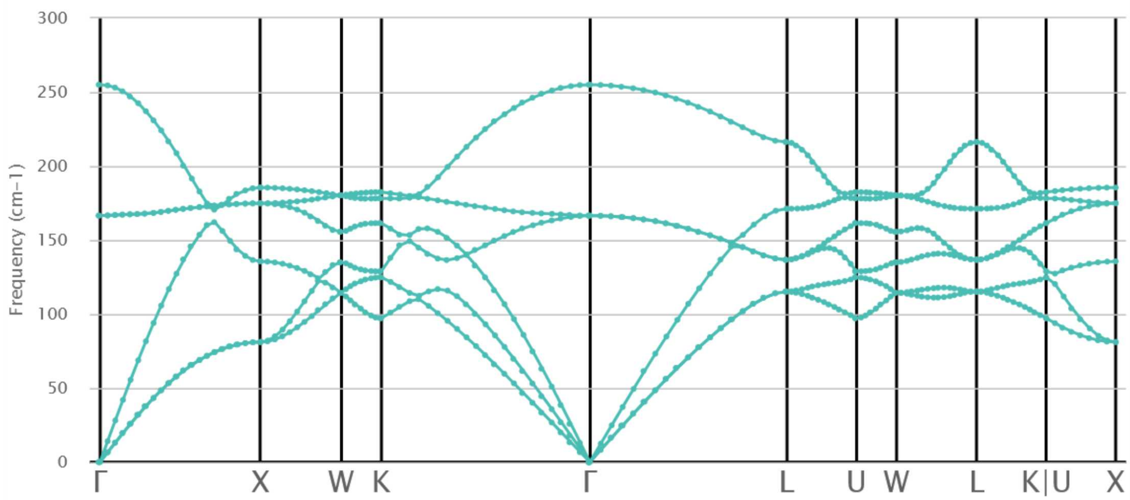
(a) Determine the number of atoms in the primitive cell and in the conventional unit cell

(b) Determine the speed of sound along [100] and [111]

(c) What is the shortest phonon wavelength possible in this crystal?

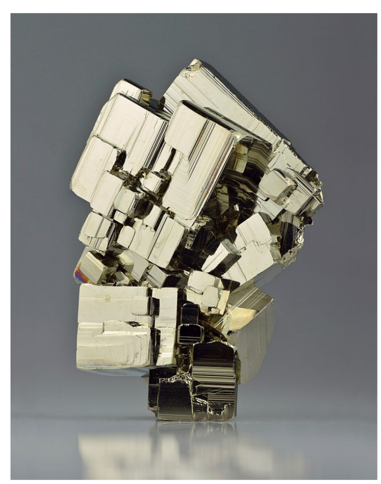
(d) Determine the occupation of the LO mode at $q = 0$ at 300 K

Hint: the drawing of the Brillouin zone and the notation of high-symmetry points for the fcc lattice can be found in textbooks or on the Bilbao server. Note that the q-path is not drawn to the scale in this spectrum.



7.2. Packing phonons into a Debye sphere (6 P)

Consider a crystal of pyrite, commonly known as "fool's gold" (FeS_2, space group $Pa\bar{3}$).



(a) How many phonon modes does it feature? How many modes should one expect in real gold?

(b) Debye model replaces full phonon spectrum with three acoustic modes that are considered within a sphere of the radius q_D instead of the first Brillouin zone. Determine the value of q_D for pyrite. How many reciprocal lattice points are contained within the Debye sphere?

(c) Speed of sound in pyrite is $v_s = 8.02$ km/s. Use this sound velocity in the linear approximation of the Debye model, $\omega = v_s\, q$, to determine the Debye temperature.

(d) Determine the high-temperature (Dulong-Petit) limit of the heat capacity. How much does heat capacity (C_V) of pyrite deviate from the Dulong-Petit limit at 300 K?

7.3. Seeing phonons with light (7 P)

Your boss wants you to study phonons in germanium and offers two experimental techniques to this end, inelastic x-ray scattering (IXS) and Brillouin light scattering (BLS). The latter is an inelastic scattering experiment performed with the visible light. Because of the longer wavelength, it covers the region around $q = 0$ only and probes acoustic phonons at low values of q.

(a) Which q-range can you access with IXS using the wavelength of 0.4 Å and with BLS using the green laser (520 nm)?

Hint: remember the Ewald sphere

(b) How many phonon modes do you expect to observe with IXS at $\mathbf{q} = (2, 0, 0)$ and $\mathbf{q} = (1.33, 0, 0)$. [Both vectors are given in units of the respective reciprocal-lattice parameter $2\pi/a$]

Hint: remember about the LO-TO splitting

(c) You measure BLS with the green laser in the perpendicular geometry (90° angle between the incident and scattered light) and observe the peaks at $\nu = 8.3$ GHz and 14.0 GHz. Determine velocities of the corresponding acoustic waves. Which one is transverse and which one is longitudinal?

(d) Determine the bulk modulus and shear modulus of germanium assuming it is an isotropic medium.