Mid-term test of Condensed Matter Physics - December 17th 2021
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Exercise 1. Figure 1 (a) shows the diffraction pattern obtained with a sample of an elemental crystal featuring cubic symmetry, by means of the powder (or Debye-Scherrer) method, using a radiation with wavelength $\lambda = 0.1542\,\text{nm}$.

1. [8 points] Determine the Bravais lattice type of the sample and the lattice parameter a of the conventional cubic cell, obtained as the average of the values calculated from each peak. In addition, associate to each peak the corresponding Miller indices (hkl).

2. [7 points] Figure 1 (b) shows the phonon dispersion curves of the same crystal along a high-symmetry direction of the first Brillouin zone (along this direction, the transverse sound modes are degenerate). Determine the effective elastic constants of the lattice, K_ℓ and K_t, assuming that the mass associated to a Bravais lattice point is $M = 3.053\times10^{-25}\,\text{kg}$ for both longitudinal and transverse modes.

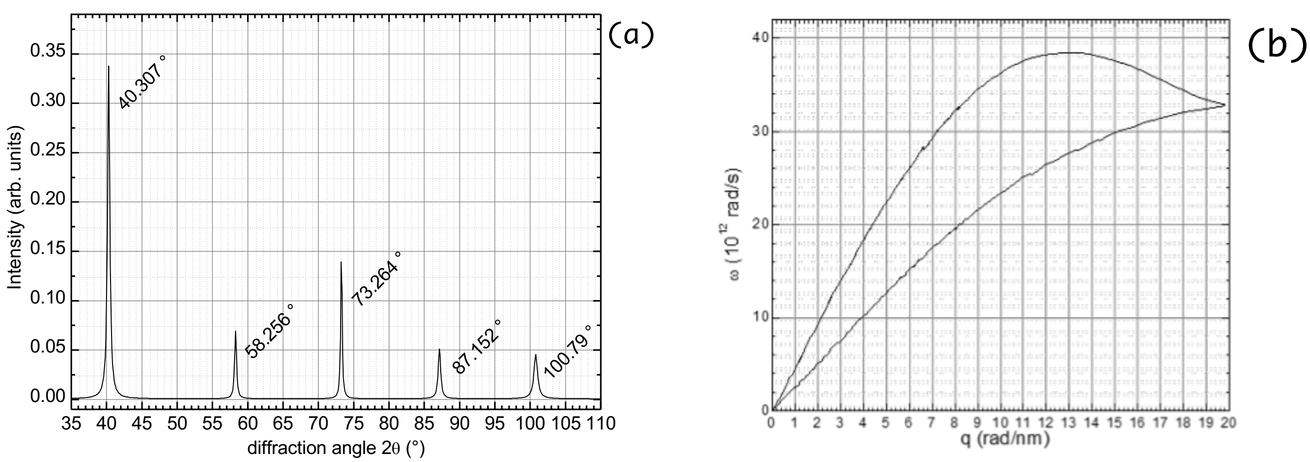

Fig. 1.

Exercise 2. Fluorite (calcium fluoride, CaF_2) forms fcc crystals, has molar mass $\mu = 7.81\times10^{-2}\,\text{kg/mol}$, and density $\varrho = 3.18\times10^3\,\text{kg/m}^3$. The velocity of sound in fluorite (averaged with respect to the directions) is $c_\ell = 6.50\times10^3\,\text{m/s}$ and $c_\text{t} = 3.98\times10^3\,\text{m/s}$, for longitudinal and transverse modes, respectively. Adopt a scheme where the optical phonons are described within the Einstein model and the acoustic phonons are described within the Debye model.

1. [3 points] Determine the number of optical branches that are observed when probing the phonon spectrum of fluorite.

2. [7 points] Determine the side a of the conventional fcc unit cell, the Debye wave vector q_D, the average sound velocity c_D, and the Debye temperature of sound modes Θ_D of fluorite.

3. [5 points] Calculate the specific heat c_v of fluorite at a temperature $T = 1\,\text{K}$, assuming that the contribution of the optical modes can be neglected altogether.

[Useful constants: $\hbar = 1.055\times10^{-34}\,\text{J}\cdot\text{s}$ (Planck's constant), $N_\text{A} = 6.02\times10^{23}\,\text{mol}^{-1}$ (Avogadro's constant), $\kappa_\text{B} = 1.38\times10^{-23}\,\text{J/K}$ (Boltzmann's constant)].

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Exercise 1.

1. Considering the plane spacing from the Bragg law $d = \lambda/(2\sin\theta)$, where $d = a/\sqrt{h^2+k^2+l^2}$, one obtains the following table:

n	2ϑ (°)	d (nm)	$(d_n/d_1)^2$ n=1,...,5	hkl	ratio	a (nm)
1'	40.307	0.22378	1.00000	100	1/1	0.22378
1	40.307	0.22378	1.00000	110	2/2	0.31647
2'	58.256	0.15839	1.99603	110	2/1	0.22400
2	58.256	0.15839	1.99603	200	4/2	0.31679
3'	73.264	0.12922	2.99921	111	3/1	0.22382
3	73.264	0.12922	2.99921	211	6/2	0.31651
4'	87.152	0.11185	4.00286	200	4/1	0.22370
4	87.152	0.11185	4.00286	220	8/2	0.31636
5'	100.79	0.10007	5.00071	210	5/1	0.22376
5	100.79	0.10007	5.00071	310	10/2	0.31645

According to the lattice plane selection rules

$\{hkl\}$	$N = h^2+k^2+l^2$	Multiplicity	cubic	bcc	fcc
100	1	6	✓		
110	2	12	✓	✓	
111	3	8	✓		✓
200	4	6	✓	✓	✓
210	5	24	✓		
211	6	24	✓	✓	
220	8	12	✓	✓	✓
221	9	24	✓		
300	9	6	✓		
310	10	24	✓	✓	
311	11	24	✓		✓
222	12	8	✓	✓	✓
⋮	⋮				

we find that the crystal is compatible with either a BCC or a SC Bravais lattice. The average lattice constant is $a = 0.3165\,\mathrm{nm}$ (BCC) or $a' = 0.2238\,\mathrm{nm}$ (SC). The two lattices become distinguishable when seven Bragg peaks are considered.

2. Taking the slope of the curves we obtain the sound velocities $v_\ell = 4590\,\mathrm{m/s}$ and $v_\mathrm{t} = 2553\,\mathrm{m/s}$. Then, $K_s = M(v_s/a)^2$, hence $K_\ell = 64.2\,\mathrm{N/m}$ and $K_\mathrm{t} = 19.9\,\mathrm{N/m}$ in the BCC case, or $K'_\ell = 128.4\,\mathrm{N/m}$ and $K'_\mathrm{t} = 39.8\,\mathrm{N/m}$ in the SC case.

Exercise 2.

1. The lattice of fluorite hosts a $p = 3$ atom basis. Therefore, the number of optical modes of fluorite is $3p - 3 = 6$.
2. In a conventional fcc unit cell there are four CaF_2 molecules, each having a mass μ/N_A, hence

$$\varrho = \frac{4\mu}{N_\mathrm{A} a^3} \qquad \Rightarrow \qquad a = \left(\frac{4\mu}{N_\mathrm{A}\,\varrho}\right)^{1/3} = 5.46 \times 10^{-10}\,\mathrm{m}.$$

The density of lattice sites in a fcc lattice is $n = 4/a^3$, hence the Debye wave vector of fluorite is

$$q_\mathrm{D} = \frac{\left(24\,\pi^2\right)^{1/3}}{a} = 1.13 \times 10^{10}\,\mathrm{m}^{-1}.$$

The average sound velocity within the Debye model is

$$c_\mathrm{D} = \left[\frac{1}{3}\left(\frac{1}{c_\ell^3} + \frac{2}{c_\mathrm{t}^3}\right)\right]^{-1/3} = 4.39 \times 10^3\,\frac{\mathrm{m}}{\mathrm{s}}.$$

Finally, the Debye temperature of the sound modes is

$$\Theta_\mathrm{D} = \frac{\hbar c_\mathrm{D} q_\mathrm{D}}{\kappa_\mathrm{B}} = 379\,\mathrm{K}.$$

3. Since $\Theta_\mathrm{D} \gg T = 1\,\mathrm{K}$, the specific heat can be calculated using the low-temperature asymptotic expression

$$c_\mathrm{v} = \frac{48\,\pi^4}{5}\,\frac{\kappa_\mathrm{B}}{a^3}\left(\frac{T}{\Theta_\mathrm{D}}\right)^3 = 1.46\,\frac{\mathrm{J}}{\mathrm{K}\cdot\mathrm{m}^3}.$$