Mid-term assessment test of Condensed Matter Physics - November 19th 2019
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Exercise 1: X ray scattering.

Cesium chloride (CsCl) crystallizes in a simple cubic lattice with a basis consisting of a Cl ion at $\mathbf{d}_1 = (0,0,0)$ and a Cs ion at the center of the cubic cell $\mathbf{d}_2 = a\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$, with $a = 0.412\,\mathrm{nm}$.

1. Determine the first 8 deflection angles $\phi = 2\theta$, measured with respect to the incident beam direction, for which diffraction peaks are observed on a detector using the powder or Debye-Scherrer method. The wavelength of the x-ray beam is $\lambda = 0.103\,\mathrm{nm}$. List the angles in order of increasing magnitude of the corresponding reciprocal lattice vector, $|\boldsymbol{K}|$, and associate each angle with the corresponding families of lattice planes.

2. Say which peaks are more intense assuming that the atomic form factor f can be put equal to Z (i.e., the atomic number) times the amplitude A of the wave scattered from one electron. Indicate with f_{Cl} and f_{Cs} the atomic form factors of Cl and Cs, respectively.

3. Which peaks would disappear if $f_{\mathrm{Cl}} = f_{\mathrm{Cs}}$? Why?

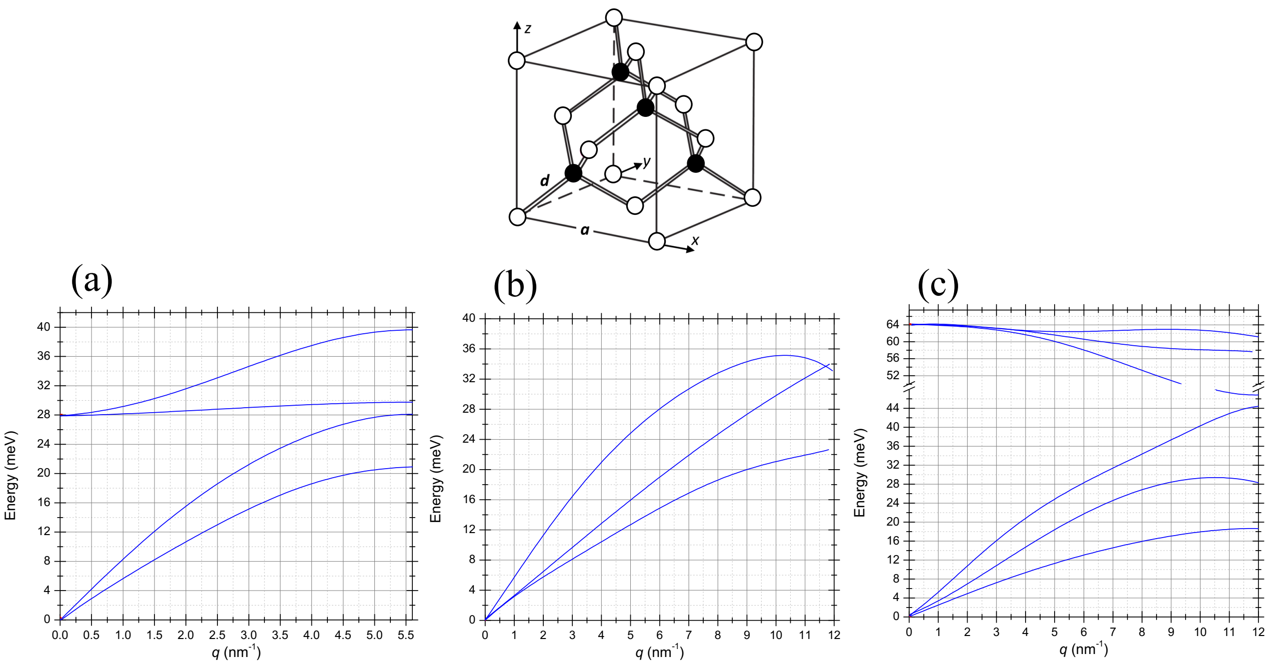

Fig. 1.

Exercise 2: Phonons.

Silicon (Si) is a face-centered cubic (fcc) lattice with two-atom basis that can be regarded as two interpenetrating fcc primitive lattices displaced by $\boldsymbol{d} = \frac{a}{4}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})$, where $a = 0.543\,\mathrm{nm}$ is the side of the conventional unit cell (see the topmost panel in the figure above; black atoms indicate the second atom of the basis) and $\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}$ are the Cartesian reference unit vectors.

1. Calculate the volume density of Si atoms (i.e., number of atoms/m^3) in the lattice.

1. Say which of the phonon dispersions (along a generic direction in the first Brillouin zone), displayed in panels (a), (b) and (c) of the figure, best describes silicon and explain why. Estimate from the correct graph the velocities of the sound modes of Si.

3. Based on the pertinent dispersion curves, estimate the Debye average sound velocity $\langle v \rangle$ and the Debye temperature Θ_D of silicon.

[Note that $1\,\mathrm{eV}$ corresponds to an energy of 1.60×10^{-19} J; the Boltzmann constant is $\kappa_B = 1.38 \times 10^{-23}\,\mathrm{J{\cdot}K^{-1}}$; the Planck constant is $\hbar = 1.055 \times 10^{-34}\,\mathrm{J{\cdot}s}$].

Solution of the written exam
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Exercise 1.

1. Since in a simple cubic lattice

$$\phi = 2\arcsin\left(\frac{|\boldsymbol{K}|}{2\kappa}\right) = 2\arcsin\left(\frac{\lambda}{2a}\sqrt{h^2+k^2+l^2}\right),$$

where $\kappa = \frac{2\pi}{\lambda}$, $|\boldsymbol{K}| = \frac{2\pi}{a}\sqrt{h^2+k^2+l^2}$, with integer h,k,l, and $\frac{\lambda}{2a} = \frac{1}{8}$, we find

peak #	h	k	l	$h^2+k^2+l^2$	ϕ (deg)
1	1	0	0	1	14.36
2	1	1	0	2	20.36
3	1	1	1	3	25.01
4	2	0	0	4	28.96
5	2	1	0	5	32.46
6	2	1	1	6	35.66
7	2	2	0	8	41.41
8	$\{$ 2 / 3	2 / 0	1 / 0	9	44.05

2. The resulting scattered amplitude is

$$I = A\left|f_{\rm Cl}\,{\rm e}^{i0} + f_{\rm Cs}\,{\rm e}^{i\pi(h+k+l)}\right|^2 = A\left|f_{\rm Cl} + (-1)^{h+k+l}f_{\rm Cs}\right|^2 \quad (1)$$

The scattered amplitude is maximum ($\propto |f_{\rm Cl}+f_{\rm Cs}|$) whenever $h+k+l$ is even (peaks # 2, 4, 6, 7), and minimum ($\propto |f_{\rm Cl}-f_{\rm Cs}|$) whenever $h+k+l$ is odd (peaks # 1, 3, 5, 8).

3. If $f_{\rm Cl} = f_{\rm Cs}$ the peaks with odd $h+k+l$ (peaks # 1, 3, 5, 8) would disappear. In this case, indeed, the given lattice would turn into a bcc Bravais lattice, and the reciprocal lattice described by a cubic lattice with even $h+k+l$ is a fcc, as expected.

Exercise 2.

1. For Si, we have 8 corner lattice points, 6 face centered points, and 2 atoms. Thus Volume density $= 8/(0.543\times 10^{-9})^3 = 5.00\times 10^{28}\,\mathrm{m}^{-3}$.

2. Graph (c) accounts best for the Si lattice. Graph (a) refers to a square lattice with a two-atom basis. Graph (b) is the dispersion curve of Al (a single-atom fcc).

The velocities of the three acoustic branches are defined by the ratios $v_i = E_i/(\hbar q)$ calculated in the linear region of the dispersion curves, say at $q = 2.2\,\mathrm{nm}^{-1}$. One obtains: $E_1 = 5.40\,\mathrm{meV}$ and $v_1 = 3729\,\mathrm{m/s}$ (first transverse acoustic mode); $E_2 = 8.00\,\mathrm{meV}$ and $v_2 = 5525\,\mathrm{m/s}$ (second transverse acoustic mode); $E_3 = 12.0\,\mathrm{meV}$ and $v_3 = 8287\,\mathrm{m/s}$ (longitudinal acoustic mode).

3. The average velocity in the Debye model is

$$\langle v\rangle = \left[\frac{1}{3}\left(\frac{1}{v_1^3}+\frac{1}{v_2^3}+\frac{1}{v_3^3}\right)\right]^{-1/3} = 4809\,\mathrm{m/s}.$$

Then

$$\Theta_D = \frac{\hbar}{\kappa_B}\left(6\pi^2 n\right)^{1/3}\langle v\rangle = 419\,\mathrm{K},$$

where $n = 2.5\times 10^{28}\,\mathrm{m}^{-3}$ is the unit cell volume density (number of unit cells per unit volume).