

Solutions, Exam TFY4220 Solid state physics spring 2021

Task 1 CsCl

Version 1:

What are the constituents of the *basis* of the CsCl structure?

Answer: 1 Cs⁺, 1 Cl⁻ ion.

Version 2:

What is the *crystal structure* for the CsCl structure?

Answer: Simple cubic

Version 3:

What is the *average form factor of the basis* of the CsCl structure?

Answer: $0.5(f_{\text{Cs}} + f_{\text{Cl}})$

Task 2 Lattice spacing

Version 1:

A diffraction signal is measured at a scattering angle $2\theta = 4.32^\circ$ using X-ray radiation with a wavelength of $1.542 \text{ \AA}$. What is the corresponding lattice spacing d ?

$$n\lambda = 2d \sin \theta$$

$$d = \frac{\lambda}{2 \sin \theta}$$

$$1.542/2/\sin(4.32/2) = 20.8913, \underline{20.5 \text{ \AA}}$$

Version 2:

A diffraction signal is measured at a scattering angle $2\theta = 4.32^\circ$ using X-ray radiation with a wavelength of $1.566 \text{ \AA}$. What is the corresponding lattice spacing d ?

$$n\lambda = 2d \sin \theta$$

$$1.566/2/\sin(4.32/2) = \underline{20.8 \text{ \AA}}$$

Version 3:

A diffraction signal is measured at a scattering angle $2\theta = 43.2^\circ$ using X-ray radiation with a wavelength of $1.542 \text{ \AA}$. What is the corresponding lattice spacing d ?

$$1.542/2/\sin(43.2/2) = 2.0944, \underline{2.09 \text{ \AA}}$$

Version 4:

A diffraction signal is measured at a scattering angle $2\theta = 43.2^\circ$ using X-ray radiation with a wavelength of $1.665 \text{ \AA}$. What is the corresponding lattice spacing d ?

$$1.665/2/\sin(43.2/2) = 2.2615, \underline{2.26 \text{ \AA}}$$

Task 3 Omega_max

Version 1

Consider the 1d monatomic chain in the harmonic lattice model as described in the lectures. Given that the mass $M = 32 \text{ u}$ and the force constant $\gamma = 1.0 \text{ N/m}$. What is the maximum frequency ω that can propagate in the lattice?

$$\text{Solution: } \sqrt{4\gamma/M} = \omega_{\max}$$

$$M = 32 \cdot 1.66 \cdot 10^{-27} \text{ kg}$$

$$\omega_{\max} = 2\sqrt{\gamma/M} = 8.67 \cdot 10^{12}$$

Answer: 8.7 THz.

Version 2

Consider the 1d monatomic chain in the harmonic lattice model as described in the lectures. Given that the mass $M = 42 \text{ u}$ and the force constant $\gamma = 1.0 \text{ N/m}$. What is the highest frequency ω that can propagate in the lattice?

$$\text{Solution: } \sqrt{4\gamma/M} = \omega_{\max}$$

$$M = 42 \cdot 1.66 \cdot 10^{-27} \text{ kg}$$

$$\omega_{\max} = 2\sqrt{\gamma/M} = 7.57 \cdot 10^{12}$$

Answer: 7.6 THz.

Task 4 Fermi energy

Kittel eq. 8.37: $D(E) = \frac{8\pi\sqrt{2}m_e^{*3/2}}{h^3} \sqrt{E - E_c}$

Version 1:

Assume a semiconductor piece measuring $10 \times 100 \times 100 \text{ nm}^3$. The effective electron mass is $1.12 m_e$. What is the number of states 0.1 eV above the conduction band edge?

$$\begin{aligned} m_{\text{eff}} &= 1.12 * 9.11\text{e-}31 && \% \text{ kg.} \\ \text{sqrtE_Ec} &= \text{sqrt}(0.1 * 1.6\text{e-}19) && \% \text{ sqrt(J)} \\ h &= 6.626\text{e-}34 && \% \text{ Js} \end{aligned}$$

$$D = 8 * \pi * \text{sqrt}(2) * m_{\text{eff}}^{3/2} * \text{sqrtE_Ec} / h^3 \quad \% = 1.59\text{e}46 \text{ m}^{-3} \text{ J}^{-1}$$

Number of states per unit energy:

$$1.59\text{e}46 * 10\text{e-}9 * 100\text{e-}9 * 100\text{e-}9 = 1.59\text{e}24 \text{ J}^{-1} = \underline{2.54\text{e}5 \text{ eV}^{-1}}$$

Version 2:

Assume a semiconductor piece measuring $10 \times 100 \times 100 \text{ nm}^3$. The effective electron mass is $1.12 m_e$. What is the number of states 0.2 eV above the conduction band edge?

$$\begin{aligned} m_{\text{eff}} &= 1.12 * 9.11\text{e-}31 && \% \text{ kg.} \\ \text{sqrtE_Ec} &= \text{sqrt}(0.2 * 1.6\text{e-}19) && \% \text{ sqrt(J)} \\ h &= 6.626\text{e-}34 && \% \text{ Js} \end{aligned}$$

$$D = 8 * \pi * \text{sqrt}(2) * m_{\text{eff}}^{3/2} * \text{sqrtE_Ec} / h^3 \quad \% = 2.25\text{e}46 \text{ m}^{-3} \text{ J}^{-1}$$

Number of states per unit energy:

$$2.25\text{e}46 * 10\text{e-}9 * 100\text{e-}9 * 100\text{e-}9 = 2.25\text{e}24 \text{ J}^{-1} = \underline{3.60\text{e}5 \text{ eV}^{-1}}$$

Version 3:

Assume a semiconductor piece measuring $10 \times 10 \times 100 \text{ nm}^3$. The effective electron mass is $1.04 m_e$. What is the number of states 0.1 eV above the conduction band edge?

$$\begin{aligned} m_{\text{eff}} &= 1.04 * 9.11\text{e-}31 && \% \text{ kg.} \\ \text{sqrtE_Ec} &= \text{sqrt}(0.1 * 1.6\text{e-}19) && \% \text{ sqrt(J)} \\ h &= 6.626\text{e-}34 && \% \text{ Js} \end{aligned}$$

$$D = 8 * \pi * \text{sqrt}(2) * m_{\text{eff}}^{3/2} * \text{sqrtE_Ec} / h^3 \quad \% = 1.43\text{e}46 \text{ m}^{-3} \text{ J}^{-1}$$

Number of states per unit energy:

$$1.43\text{e}46 * 10\text{e-}9 * 10\text{e-}9 * 100\text{e-}9 = 1.43\text{e}23 \text{ J}^{-1} = \underline{2.28\text{e}4 \text{ eV}^{-1}}$$

Task 5. Fermi wave vector

Kittel eq. 6.16: $k_F = \left(\frac{3\pi^2 N}{V} \right)^{1/3}$

Version 1:

Consider a BCC material with one conduction electron per primitive cell, in the free electron Fermi gas model. The lattice parameter $a = 4.2 \text{ \AA}$.

What is the magnitude of the Fermi wave vector?

$$N = 2$$

$$a = 4.2 \times 10^{-10}$$

$$V = a^3$$

$$k_F = (3\pi^2 N/V)^{1/3} \quad \% = 9.28 \times 10^9 \text{ m}^{-1} = \underline{0.93 \text{ \AA}^{-1}}$$

Version 2:

Consider an FCC material with one conduction electron per primitive cell, in the free electron Fermi gas model. The lattice parameter $a = 4.2 \text{ \AA}$.

What is the magnitude of the Fermi wave vector?

$$N = 4$$

$$a = 4.2 \times 10^{-10}$$

$$V = a^3$$

$$k_F = (3\pi^2 N/V)^{1/3} \quad \% = 1.169 \times 10^{10} \text{ m}^{-1} = \underline{1.17 \text{ \AA}^{-1}}$$

Version 3:

Consider a BCC material with one conduction electron per primitive cell, in the free electron Fermi gas model. The lattice parameter $a = 5.2 \text{ \AA}$.

What is the magnitude of the Fermi wave vector?

$$N = 2$$

$$a = 5.2 \times 10^{-10}$$

$$V = a^3$$

$$k_F = (3\pi^2 N/V)^{1/3} \quad \% = 7.495 \times 10^9 \text{ m}^{-1} = \underline{0.75 \text{ \AA}^{-1}}$$

Task 6 Lattice plane atomic density

Version 1:

A material with a bcc unit cell and one atom per Bravais point has a lattice constant of 0.288 nm.

What is the number density of atoms in the (110) plane?

$$\begin{aligned} N &= 2 \text{ \% atoms per rectangle} \\ a &= 0.288 \times 10^{-6} \text{ \% mm} \\ b &= \sqrt{2} * a \\ \rho &= N/(a*b) \text{ \%} = \underline{17 \times 10^{12} \text{ mm}^{-2}} \end{aligned}$$

Version 2:

A material with a bcc unit cell and one atom per Bravais point has a lattice constant of 0.228 nm. What is the number density of atoms in the (110) plane?

$$\begin{aligned} N &= 2 \text{ \% atoms per rectangle} \\ a &= 0.228 \times 10^{-6} \text{ \% mm} \\ b &= \sqrt{2} * a \\ \rho &= N/(a*b) \text{ \%} = \underline{27 \times 10^{12} \text{ mm}^{-2}} \end{aligned}$$

Task 7 Volume of reciprocal unit cell

Version 1:

Assuming that the primitive translation vectors of a lattice are given by

$$\mathbf{a} = \sqrt{2}(\mathbf{x} - \mathbf{y}); \mathbf{b} = \sqrt{2}(\mathbf{x} + \mathbf{y}); \mathbf{c} = 3\mathbf{z}.$$

What is the corresponding volume of the reciprocal space unit cell?

Answer:

The tedious way is to calculate all the reciprocal space vectors, and then calculate the volume by $V^* = \mathbf{a}^* \cdot (\mathbf{b}^* \times \mathbf{c}^*)$

It is faster to note that $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are orthogonal, with $a = b = 2, c = 3$.

Then, in reciprocal space, $a^* = 2\pi/a = \pi, b^* = 2\pi/b = \pi, c^* = 2\pi/c = 2\pi/3$.

$$\text{In reciprocal space, } V^* = a^* b^* c^* = \pi \cdot \pi \cdot 2\pi / 3 = \frac{2}{3} \pi^3.$$

Alternatively, a theorem (see Kittel, problem 2.4) states that $V^* = (2\pi)^3/V$. With $V = \mathbf{a} \cdot \mathbf{b} \cdot \mathbf{c} = abc = 2 \cdot 2 \cdot 3 = 12$, this gives $8\pi^3/12 = \underline{2\pi^3/3}$.

Version 2:

Assuming that the primitive translation vectors of a lattice are given by

$$\mathbf{a} = \sqrt{3}(\mathbf{x} - \mathbf{y}); \mathbf{b} = \sqrt{3}(\mathbf{x} + \mathbf{y}); \mathbf{c} = 3\mathbf{z}.$$

What is the corresponding volume of the reciprocal space unit cell?

Answer:

Here, $a^* = 2\pi/a = 2\pi/\sqrt{6}, b^* = 2\pi/b = 2\pi/\sqrt{6}, c^* = 2\pi/c = 2\pi/3$.

$$\text{In reciprocal space: } V^* = a^* b^* c^* = (2\pi / \sqrt{6})^2 (2\pi / 3) = \underline{\underline{\frac{4}{9} \pi^3}}.$$

Version 3:

Assuming that the primitive translation vectors of a lattice are given by

$$\mathbf{a} = \sqrt{3}(\mathbf{x} - \mathbf{y}); \mathbf{b} = \sqrt{3}(\mathbf{x} + \mathbf{y}); \mathbf{c} = 2\mathbf{z}.$$

What is the corresponding volume of the reciprocal space unit cell?

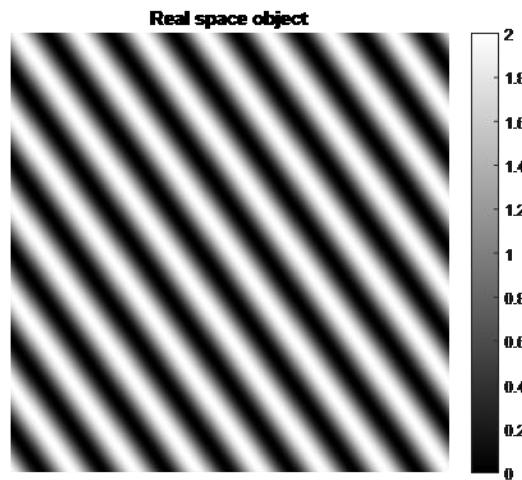
Answer:

Here, $a^* = 2\pi/a = 2\pi/\sqrt{6}, b^* = 2\pi/b = 2\pi/\sqrt{6}, c^* = 2\pi/c = \pi$.

$$\text{In reciprocal space: } V^* = a^* b^* c^* = (2\pi / \sqrt{6})^2 \pi = \underline{\underline{\frac{2}{3} \pi^3}}.$$

(Task 8 – 17 in random order)**Task 8-I. FT of linear grating**

A real space density distribution (extending to infinity in all directions) is shown as the "Real space object":



The density variation $\rho(x,y)$ is given by the square of a sinusoidal variation on a flat background, ensuring that the density is everywhere ≥ 0 .

Which of the suggested patterns depicts the corresponding absolute square ("power spectrum") of the Fourier transform, i.e., $|FT(\rho)|^2$?

Answer:

A harmonic oscillation has only one frequency f_0 . The (complex) Fourier transform returns the positive and negative frequencies ($\pm f_0$) with equal weight, symmetrically about the origin, with the direction corresponding to the wave front normal. In addition, the constant background corresponds to a Dirac δ -function at the origin of k -space (zero frequency or «dc-term»).

Correct answer: a.

Task 8-II. Max phonon v_g

It can be shown that the dispersion relation for phonons on a 1D string with next nearest neighbours included is given by

$$\omega^2 = \frac{4}{M} \left(C_1 \sin^2 \frac{ka}{2} + C_2 \sin^2 ka \right)$$

Here, M is the mass of the atoms, C_1 and C_2 are force constants, a denotes the interatomic spacing and k is the wave vector.

Now assume $C_2 = \frac{1}{2} C_1$. The dispersion relation is plotted in the figure (red broken line). For comparison, the standard nearest neighbour dispersion relation with the same values for C_1 and M is also plotted.

What is the limiting value of the group velocity for large wavelengths?

$$\begin{aligned} \omega^2 &= \frac{4}{M} \left(C_1 \sin^2 \frac{ka}{2} + C_2 \sin^2 ka \right) \rightarrow \\ \omega^2 &\approx \frac{4}{M} \left(C_1 \frac{k^2 a^2}{4} + C_2 k^2 a^2 \right) = \frac{4k^2 a^2}{M} \left(\frac{C_1}{4} + \frac{C_1}{2} \right) = \frac{4k^2 a^2 C_1}{M} \frac{3}{4} \\ \omega &= \sqrt{\frac{3k^2 a^2 C_1}{M}} = ka \sqrt{\frac{3C_1}{M}} \\ v_g &= \frac{\partial \omega}{\partial k} = a \sqrt{\frac{3C_1}{M}} \end{aligned}$$

Task 8-III. Diffraction, morphology

In a diffraction experiment with monochromatic X-ray radiation, an unknown substance is measured. A point detector (sensor) is used to measure the intensity as function of scattering angle 2θ .

First, a scan is done of the scattering angle 2θ , giving a diffraction pattern $I(2\theta)$ consisting of many sharp Bragg peaks.

Second, the point detector is kept stationary at a position $2\theta_0$ which gave a strong measured intensity in the first scan. While the sample is rotated 360° , the scattered intensity measured by the detector shows only a few sharp diffraction points with low intensity in-between.

Which alternative can explain these observations?

Answer: single crystal.

Task 8-IV. Phonon collision

In a 1D phonon annihilation process two transverse acoustic phonons combine to give one longitudinal acoustic phonon. The dispersion relations for transverse and longitudinal phonons are

$$\omega_{TA} = \omega_0 |\sin(ka/2)|$$

and

$$\omega_{LA} = 2\omega_0 |\sin(ka/2)|$$

For which of the following acoustic phonon wave vectors k_1 and k_2 is the process allowed?

Answer:

$k_1 = k_2 = 2\pi/3a$ simultaneously satisfies both conservation of crystal momentum and energy:

Crystal momentum before: $k_1 + k_2$

Crystal momentum after: $k_1 + k_2 = 2 \cdot 2\pi/3a = 4\pi/3a$, equivalent to $-2\pi/3a$.

Energy before: $2\omega_0 |\sin(ka/2)| = 2\omega_0 |\sin(\pi/3)| = \omega_0 \sqrt{3}$

Energy after: $\omega_{LA} = 2\omega_0 |\sin(ka/2)| = 2\omega_0 |\sin(\frac{-2\pi}{3a} \frac{a}{2})| = 2\omega_0 |\sin(\frac{-\pi}{3})| = \omega_0 \sqrt{3}$

(Similar calculations show that the other alternatives are not allowed)

Task 8-V. Filling ratio

A molecular crystal consists of densely packed compact spheroid-shaped molecules with radii $r_a = r_b < r_c$. There is one molecule per unit cell. The crystal structure is hexagonal, the molecules are oriented with their long axis along the unit cell c -axis, and $c = 2r_c$. In the (a,b) -plane, the molecules are hexagonally dense packed, with $a = b = 2r_a$. What is the filling ratio (or "packing ratio") of the structure?

Answer:

Volume of hexagonal unit cell: $V = a^2 c \sin(120^\circ) = \frac{\sqrt{3}}{2} (2r_a)^2 (2r_c) = 4\sqrt{3} r_a^2 r_c =$

Volume of spheroid: $V_{sph} = \frac{4}{3} \pi r_a^2 r_c$

$$\text{Filling ratio} = \frac{V_{sph}}{V_{cell}} = \frac{\frac{4}{3} \pi r_a^2 r_c}{4\sqrt{3} r_a^2 r_c} = \frac{\pi}{3\sqrt{3}} \sim 0.60$$

Task 8-VI. Fermi pressure

Thermodynamically, the pressure is related to the energy by $p = - \left(\frac{\partial U}{\partial V} \right)_{N \text{ const}}$. One can thus

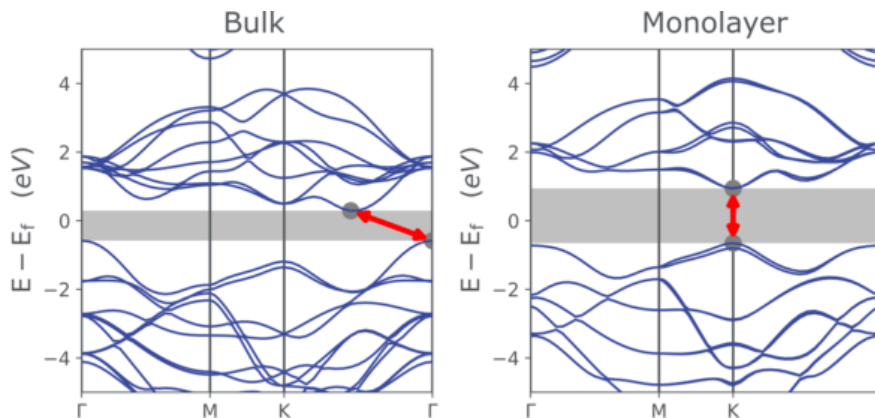
derive that because of the volume dependence of the Fermi energy, $E_F \propto \left(\frac{N}{V} \right)^{2/3}$, the electron gas exerts a pressure.

Answer:

The volume dependence of the pressure of the free electron Fermi gas is given by:

Total energy of Fermi sphere $\sim E_0 + E_F \propto V^{-2/3}$, where E_0 is the zero-point energy (a constant).

$$p = - \left(\frac{\partial E}{\partial V} \right)_N = - \frac{\partial}{\partial V} \left\{ V^{-\frac{2}{3}} \right\}_N \propto V^{-\frac{5}{3}}$$

Task 8-VII. Monolayer el. struct.

A bulk material that can be exfoliated (turned into a single molecular layer, "2D" monolayer) has electronic band structure as shown in the figure. Which statement is correct?

Answer: The monolayer bandgap is direct. Compared to the bulk, it is larger.

Interested in more info? Read <https://www.ossila.com/pages/molybdenum-disulfide-mos2>

Task 8-VII. Average electron energy

According to the free electron Fermi gas model, the density of states is proportional to the square root of the energy, $D(E)$. Considering the 20% of the electrons, i.e., $N/5$, occupying the lowest energy states, what is their average energy at $T = 0$ K?

In the expressions below, N is the number of electrons and E_F denotes the Fermi energy.

Answer:

The easy way to approach this problem is to consider just a re-scaling of the Fermi-level.

This gives immediately $\langle E_{20\%} \rangle = \frac{3}{25} E_F$

If a lengthier derivation is desired, one can for example proceed as follows.

Let $D(E)dE = A\sqrt{E}dE$, where A is a constant.

We know that $N = \int_0^{E_F} D(E)dE$ and $E_{tot} = \int_0^{E_F} ED(E)dE$.

$$N_{20\%} = \int_0^{E_F/5} D(E)dE = A \int_0^{E_F/5} E^{1/2} dE = \frac{2A}{3} (E_F/5)^{3/2} = \frac{2}{3 \cdot 5^{3/2}} A E_F^{3/2}$$

$$E_{20\%} = \int_0^{E_F/5} ED(E)dE = A \int_0^{E_F/5} E^{3/2} dE = \frac{2A}{5} (E_F/5)^{5/2} = \frac{2}{5^{7/2}} A E_F^{5/2}$$

$$\langle E_{20\%} \rangle = \frac{E_{20\%}}{N_{20\%}} = \frac{3}{25} E_F$$

Task 8-VIII. G vector

A single crystal is oriented in the orthogonal laboratory coordinate system (x,y,z), where z is the vertical direction. The crystal belongs to the monoclinic crystal system with primitive translation vectors oriented with $\mathbf{a} = ax$, $\mathbf{b} = by$ and $\mathbf{c} = c \cos(\beta)\mathbf{x} + c \sin(\beta)\mathbf{z}$. The incoming X-ray beam is directed along $\mathbf{y}$. The point detector (sensor) is placed in the (y,z) plane, and is at an angle 2θ with respect to the horizontal, as shown in the figure.

Define a reciprocal coordinate system $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$, with $\mathbf{X} \parallel \mathbf{x}$, $\mathbf{Y} \parallel \mathbf{y}$, and $\mathbf{Z} \parallel \mathbf{z}$.

Which expression gives a correct representation of the reciprocal lattice vector $\mathbf{G}_{100}$?

Answer:

$$\mathbf{G}_{100} = \mathbf{a}^* = \frac{2\pi}{V_c} \mathbf{b} \times \mathbf{c}, \quad V_c = \mathbf{a} \cdot \mathbf{b} \times \mathbf{c} = abc \sin \beta$$

$$\mathbf{b} \times \mathbf{c} = bc \langle \sin \beta, 0, -\cos \beta \rangle$$

$$\mathbf{G}_{100} = \frac{2\pi}{a} \langle 1, 0, -\cot \beta \rangle$$

Task 8-IX. Q vector

A single crystal is oriented in the orthogonal laboratory coordinate system (x,y,z), where z is the vertical direction. The crystal belongs to the monoclinic crystal system with primitive translation vectors oriented with $\mathbf{a} = ax$, $\mathbf{b} = by$ and $\mathbf{c} = c \cos(\beta)\mathbf{x} + c \sin(\beta)\mathbf{z}$. The incoming X-ray beam is directed along $\mathbf{y}$. The point detector (sensor) is placed in the (y,z) plane, and is at an angle 2θ with respect to the horizontal, as shown in the figure.

Define a reciprocal coordinate system $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$, with $\mathbf{X} \parallel \mathbf{x}$, $\mathbf{Y} \parallel \mathbf{y}$, and $\mathbf{Z} \parallel \mathbf{z}$.

Which expression gives a correct representation of the scattering vector $\mathbf{Q}$ that can be measured with the given geometry?

Answer:

$$\mathbf{k}_i = \frac{2\pi}{\lambda} \langle 0, 1, 0 \rangle, \quad \mathbf{k}_f = \frac{2\pi}{\lambda} \langle 0, \cos 2\theta, \sin 2\theta \rangle$$

$$\mathbf{Q} \equiv \mathbf{k}_f - \mathbf{k}_i = \frac{2\pi}{\lambda} \langle 0, \cos 2\theta - 1, \sin 2\theta \rangle$$

Task 18. Inverse Umklapp

Version 1

In a rectangular 2D lattice with $a = 6.90 \text{ \AA}$ and $b = 4.50 \text{ \AA}$, three phonons each having wave vector $\mathbf{k} = \langle 0.80, 0.90 \rangle \text{ \AA}^{-1}$ merge to become one phonon. (Assume that the energy is conserved).

What is the reduced zone scheme representation of the resulting phonon?

$$3\mathbf{k} = \langle 2.4, 2.7 \rangle \text{ \AA}^{-1}.$$

$$a = 6.90 \text{ \AA} \rightarrow a^* = 2\pi/6.90 \text{ \AA}^{-1} = 0.91 \text{ \AA}^{-1}. \text{ 1st BZ boundary at } 0.45 \text{ \AA}^{-1}.$$

$$b = 4.50 \text{ \AA} \rightarrow b^* = 2\pi/4.50 \text{ \AA}^{-1} = 1.40 \text{ \AA}^{-1}. \text{ 1st BZ boundary at } 0.70 \text{ \AA}^{-1}.$$

$$2.4 - 3 \cdot 0.91 = -0.33$$

$$2.7 - 2 \cdot 1.40 = -0.10$$

$$\text{Answer: } \langle -0.33, -0.10 \rangle$$

Version 2

In a rectangular 2D lattice with $a = 6.90 \text{ \AA}$ and $b = 4.60 \text{ \AA}$, four phonons each having wave vector $\mathbf{k} = \langle 0.80, 0.90 \rangle \text{ \AA}^{-1}$ merge to become one phonon. (Assume that the energy is conserved). What is the reduced zone scheme representation of the resulting phonon?

$$4\mathbf{k} = \langle 3.2, 3.6 \rangle \text{ \AA}^{-1}.$$

$$a = 6.90 \text{ \AA} \rightarrow a^* = 2\pi/6.90 \text{ \AA}^{-1} = 0.91 \text{ \AA}^{-1}. \text{ 1st BZ boundary at } 0.45 \text{ \AA}^{-1}.$$

$$b = 4.60 \text{ \AA} \rightarrow b^* = 2\pi/4.60 \text{ \AA}^{-1} = 1.37 \text{ \AA}^{-1}. \text{ 1st BZ boundary at } 0.68 \text{ \AA}^{-1}.$$

$$3.2 - 4 \cdot 0.91 = -0.44$$

$$3.6 - 3 \cdot 1.37 = -0.51$$

$$\text{Answer: } \langle -0.44, -0.51 \rangle$$

Version 3

In a rectangular 2D lattice with $a = 6.90 \text{ \AA}$ and $b = 4.60 \text{ \AA}$, two phonons each having wave vector $\mathbf{k} = \langle 0.80, 0.90 \rangle \text{ \AA}^{-1}$ merge to become one phonon. (Assume that the energy is conserved). What is the reduced zone scheme representation of the resulting phonon?

$$2\mathbf{k} = \langle 1.6, 1.8 \rangle \text{ \AA}^{-1}.$$

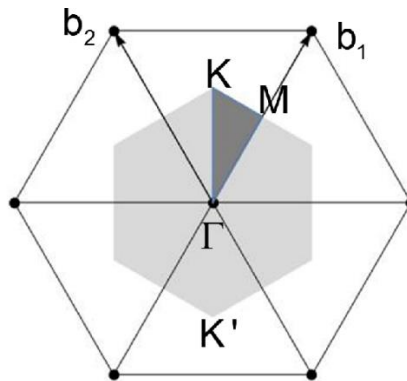
$$a = 6.90 \text{ \AA} \rightarrow a^* = 2\pi/6.90 \text{ \AA}^{-1} = 0.91 \text{ \AA}^{-1}. \text{ 1st BZ boundary at } 0.45 \text{ \AA}^{-1}.$$

$$b = 4.60 \text{ \AA} \rightarrow b^* = 2\pi/4.60 \text{ \AA}^{-1} = 1.37 \text{ \AA}^{-1}. \text{ 1st BZ boundary at } 0.68 \text{ \AA}^{-1}.$$

$$1.6 - 2 \cdot 0.91 = -0.22$$

$$1.8 - 1 \cdot 1.37 = 0.43$$

$$\text{Answer: } \langle -0.22, 0.43 \rangle$$

Task 19. Energy at 2D hex M point

Version 1

The figure shows the Brillouin zone of a 2D hexagonal lattice.

According to the free electron Fermi model, what is the energy of electrons at the M point in reciprocal space (see sketch)?

Assume $a = 2.9 \text{ \AA}$.

(Take the energy to be zero at the Brillouin zone centre).

Answer:

$$a^* = \frac{2\pi}{a_\perp} = \frac{2\pi}{a\sqrt{3}/2} = \frac{4\pi}{\sqrt{3}a}; \quad k_M = \Gamma M = \frac{a^*}{2} = \frac{2\pi}{\sqrt{3}a}; \quad E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \frac{4\pi^2}{3a^2} = \frac{h^2}{6ma^2}$$

With numbers: $E = 6.0 \text{ eV}$.

Version 2:

The figure shows the Brillouin zone of a 2D hexagonal lattice.

According to the free electron Fermi model, what is the energy of electrons at the M point in reciprocal space (see sketch)?

Assume $a = 4.1 \text{ \AA}$.

(Take the energy to be zero at the Brillouin zone centre).

$E = 3.0 \text{ eV}$

Version 3:

The figure shows the Brillouin zone of a 2D hexagonal lattice.

According to the free electron Fermi model, what is the energy of electrons at the M point in reciprocal space (see sketch)?

Assume $a = 2.5 \text{ \AA}$.

(Take the energy to be zero at the Brillouin zone centre).

$E = 8.0 \text{ eV}$

(Task 20 – 25 in random order)

Task 20-I. Fourier filtering

Figure illustrating Fourier filtering. a) Artificially generated object. b) Fourier transform squared of the object shown in (a). c) Illustration of a mask applied to the Fourier transform. d) Resulting image after inverse Fourier transformation of the masked signal.

The red crosses mark the origin of Fourier space ($k_x = k_y = 0$).

Which of the following statements is *incorrect*?

Answer: The *incorrect* statement is that the illustrated process corresponds to bright-field imaging.

Task 20-II. Basis of FCC unit cell.

A unit cell with the generic structure AB_2 is face centered cubic (FCC), with A^{2+} in the corners and the face centres, and B^- on the space diagonals at a distance of $1/4$ of the diagonal from all the corners.

Which alternative gives a correct description of the basis (associated with each Bravais lattice point) for this FCC unit cell?

Answer:

The basis is A^+ at $(1,0,0)$ (which is equivalent to $(0,0,0)$)
 B^- at $(-1/4, -1/4, -1/4)$ and $(1/4, 1/4, 1/4)$.

Task 20-III. Intensity based on form factor.

A cubic crystal structure containing two elements with atomic form factors f_A and f_B has structure factor given by

$$S_{hkl} = f_A(1 + (-1)^{h+k+l}) + f_B \exp\left(\frac{\pi}{2} i(h+k+l)\right) \cdot [1 + (-1)^{h+k} + (-1)^{k+l} + (-1)^{l+h}].$$

Which expression is proportional to the scattered *intensity* in the special case of h, k and l all odd? Assume f_A and f_B real.

Answer: For h, k, l all odd, one finds that a simplified expression for the form factor is

$$S_{hkl} = 4i(-1)^n f_B$$

The intensity is proportional to the absolute square of the structure factor, giving

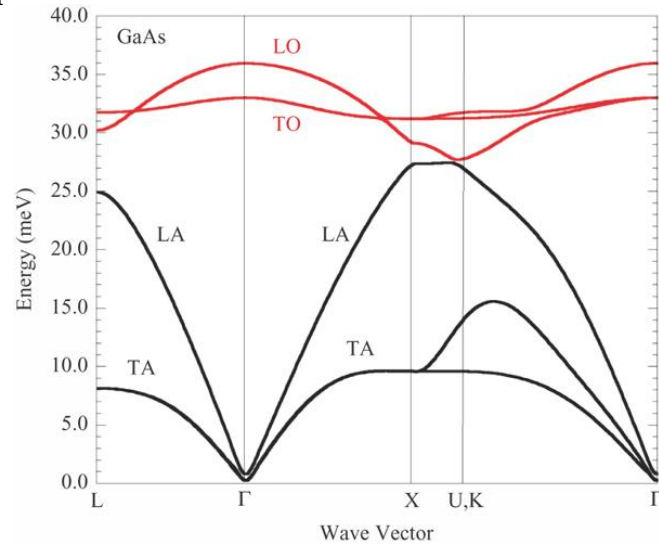
$$\underline{I_{all\ odd} = |4i(-1)^n f_B|^2 = 16 f_B^2}$$

Task 20-IV. Bloch function

A 1D electronic wave function is given by $\psi_k(x) = \exp(ikx) \exp(-B \sin^2(\sqrt{\kappa}x))$, where B and κ are constants.

Which of the expressions below satisfies the requirements for ψ_k to describe an electronic state in a periodic potential?

Answer: Both $\underline{\kappa = (\pi/a)^2}$ and $\underline{\kappa = (2\pi/a)^2}$ must be approved for this task, as these expressions give a Bloch function being a plane wave multiplied by a periodic function having the periodicity of the lattice.

Task 20-V. GaAs optics

The figure shows the dispersion relations for lattice vibrations in GaAs, which is cubic with $a = 5.65 \text{ \AA}$. Find the approximate wavelength of the most strongly absorbed electromagnetic radiation by the LO phonons.

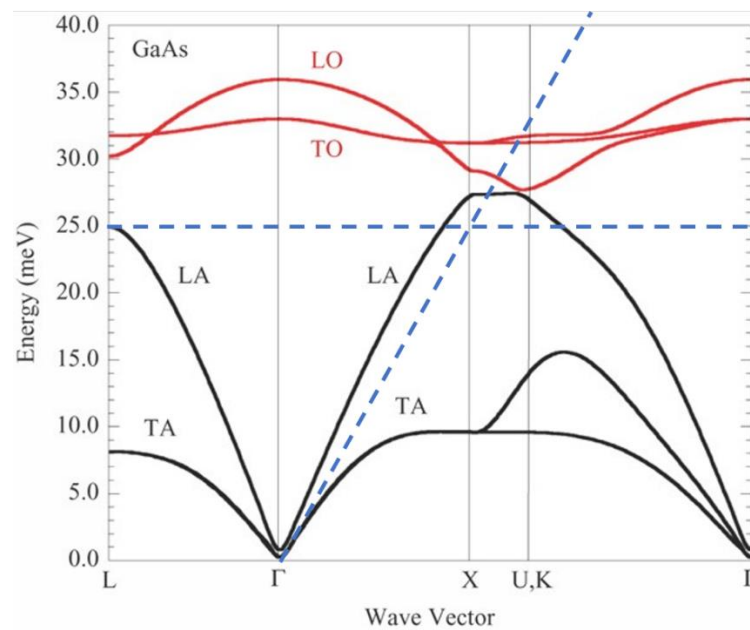
Answer:

Near the Γ point, the energy is $E = 36.0 \text{ meV} = 5.76 \times 10^{-21} \text{ J}$.

Photons with this energy have a wavelength λ , given implicitly by $E = \frac{hc}{\lambda}$

Thus, $\lambda = \frac{hc}{E} = \underline{35 \text{ }\mu\text{m}}$.

Task 20-VI. Semiconductor, speed of sound



The figure shows the dispersion relations for lattice vibrations in a semiconductor, which is cubic with $a = 5.65 \text{ \AA}$. Note that the X-point of the fcc structure is at $2\pi/a$.

Find the approximate speed of sound corresponding to the TA mode, using the indicated intersection at $E = 25.0 \text{ meV}$.

Answer:

The energy at the intersection with the X point is $25 \text{ meV} = 4.00 \times 10^{-21} \text{ J}$.

$$\Delta\omega = E / \hbar = 3.79 \times 10^{13} \text{ rad}^{-1}.$$

$$\text{X-point: } \Delta k = 2\pi/a = 2$$

$$vg = \frac{\partial\omega}{\partial k} \approx \frac{d\omega}{dk}$$

$$\underline{25 \times 10^{-3} \text{ eV} / \hbar / (2\pi / 5.65 \times 10^{-10}) = 3410 \text{ m/s.}}$$

Task 26. C_v diamond

Version 1

Diamond has a Debye temperature of about 1860 K. Estimate the heat capacity of diamond at 180 K using the Debye formalism.

$$C' = \frac{12}{5} \pi^4 N k_B (T/T_D)^3 \quad \text{Heat capacity for } N \text{ atoms}$$

$$C = N_A \cdot C'/N = \frac{12}{5} \pi^4 N k_B (T/T_D)^3 \quad \text{Heat capacity for } n \text{ moles}$$

$$N_A = 6.022 \times 10^{23};$$

$$k_B = 1.38 \times 10^{-23};$$

$$C = 12 \pi^4 / 5 \cdot k_B \cdot (180/1860)^3 \cdot N_A = 1.76 \quad \text{Answer: } 1.7 \text{ J/(mol}\cdot\text{K)}$$

Version 2

Diamond has a Debye temperature of about 1860 K. Estimate the heat capacity of diamond at 160 K using the Debye formalism.

$$C = 12 \pi^4 / 5 \cdot k_B \cdot (160/1860)^3 \cdot N_A = 1.23 \quad \text{Answer: } 1.2 \text{ J/(mol}\cdot\text{K)}$$

Version 3

Diamond has a Debye temperature of about 1860 K. Estimate the heat capacity of diamond at 140 K using the Debye formalism.

$$C = 12 \pi^4 / 5 \cdot k_B \cdot (140/1860)^3 \cdot N_A = 0.83 \quad \text{Answer: } 0.8 \text{ J/(mol}\cdot\text{K)}$$