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: $0.5(f_{Cs} + f_{Cl})$

Task 2 Lattice spacing

Version 1:
A diffraction signal is measured at a scattering angle $2\theta =$ 4.32° using X-ray radiation with a wavelength of 1.542 Å. What is the corresponding lattice spacing *d*?
$n\lambda = 2d\sin\theta$
$$d = \frac{\lambda}{2\sin\theta}$$
1.542/2/sind(4.32/2) = 20.8913, 20.5 Å

Version 2:
A diffraction signal is measured at a scattering angle $2\theta =$ 4.32° using X-ray radiation with a wavelength of 1.566 Å. What is the corresponding lattice spacing *d*?
$n\lambda = 2d\sin\theta$
1.566/2/sind(4.32/2) = 20.8 Å

Version 3:
A diffraction signal is measured at a scattering angle $2\theta =$ 43.2° using X-ray radiation with a wavelength of 1.542 Å. What is the corresponding lattice spacing *d*?
1.542/2/sind(43.2/2) = 2.0944, 2.09 Å

Version 4:
A diffraction signal is measured at a scattering angle $2\theta =$ 43.2° using X-ray radiation with a wavelength of 1.665 Å. What is the corresponding lattice spacing *d*?
1.665/2/sin(43.2/2) = 2.2615, 2.26 Å

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 u and the force constant γ = 1.0 N/m. What is the maximum frequency ω that can propagate in the lattice?

Solution: $\sqrt{(4\gamma/M)} = \omega_{max}$
$M = 32 \cdot 1.66\text{e-}27$ kg
$\omega_{max} = 2\sqrt{(\gamma/M)} = 8.67$ e12
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 u and the force constant γ = 1.0 N/m. What is the highest frequency ω that can propagate in the lattice?

Solution: $\sqrt{(4\gamma/M)} = \omega_{max}$
$M = 42 \cdot 1.66\text{e-}27$ kg
$\omega_{max} = 2\sqrt{(\gamma/M)} = 7.57$ e12
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 x 100 x 100 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?

meff = 1.12 * 9.11e-31 % kg.
sqrtE_Ec = sqrt(0.1 * 1.6e-19) % sqrt(J)
h = 6.626e-34 % Js

D = 8 * pi * sqrt(2) * meff^(3/2) * sqrtE_Ec / h^3 % = 1.59e46 m^{-3} J^{-1}

Number of states per unit energy:
1.59e46 * 10e-9*100e-9*100e-9 = 1.59e24 J^{-1} = 2.54e5 eV^{-1}

Version 2:
Assume a semiconductor piece measuring 10 x 100 x 100 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?

meff = 1.12 * 9.11e-31 % kg.
sqrtE_Ec = sqrt(0.2 * 1.6e-19) % sqrt(J)
h = 6.626e-34 % Js
D = 8 * pi * sqrt(2) * meff^(3/2) * sqrtE_Ec / h^3 % = 2.25e46 m^{-3} J^{-1}

Number of states per unit energy:
2.25e46 * 10e-9*100e-9*100e-9 = 2.25e24 J^{-1} = 3.60e5 eV^{-1}

Version 3:
Assume a semiconductor piece measuring 10 x 10 x 100 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?

meff = 1.04 * 9.11e-31 % kg.
sqrtE_Ec = sqrt(0.1 * 1.6e-19) % sqrt(J)
h = 6.626e-34 % Js

D = 8 * pi * sqrt(2) * meff^(3/2) * sqrtE_Ec / h^3 % = 1.43e46 m^{-3} J^{-1}
Number of states per unit energy:

1.43e46 * 10e-9*10e-9*100e-9 = 1.43e23 J^{-1} = 2.28e4 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 Å.

What is the magnitude of the Fermi wave vector?

N = 2
a = 4.2e-10
V = a^3
kF = (3*pi^2*N/V) ^ (1/3) % = 9.28e9 m^{-1} = 0.93 $Å^{-1}$

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 Å.

What is the magnitude of the Fermi wave vector?
N = 4
a = 4.2e-10
V = a^3
kF = (3*pi^2*N/V) ^ (1/3) % = 1.169e10 m^{-1} = 1.17 $Å^{-1}$

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 Å.

What is the magnitude of the Fermi wave vector?
N = 2
a = 5.2e-10
V = a^3
kF = (3*pi^2*N/V) ^ (1/3) % = 7.495e9 m^{-1} = 0.75 $Å^{-1}$

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?

N = 2 % atoms per rectangle
a = 0.288e-6 % mm
b = sqrt(2)*a
rho = N/(a*b) % = 17e12 mm^{-2}

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?

N = 2 % atoms per rectangle
a = 0.228e-6 % mm
b = sqrt(2)*a
rho = N/(a*b) % = 27e12 mm^{-2}

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 **a**, **b**, **c** are orthogonal, with $a = b = 2$, $c = 3$.

Then, in reciprocal space, $a^* = 2\pi/a = \pi$, $b^* = 2\pi/b = \pi$, $c^* = 2\pi/c = 2\pi/3$.
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 $8\pi^3/12 = 2\pi^3/3$.

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

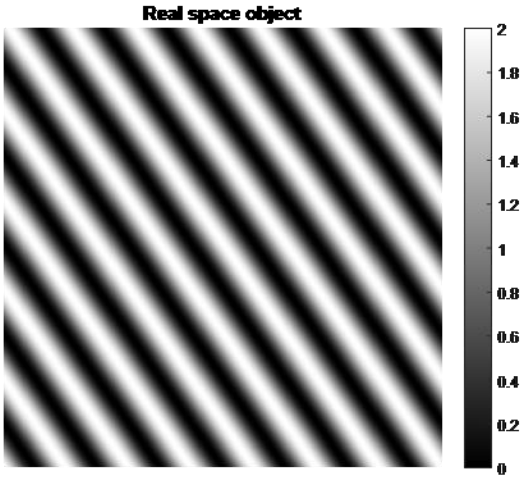
Version 3:
Assuming that the primitive translation vectors of a lattice are given by
$\mathbf{a} = \sqrt{3}(\mathbf{x} - \mathbf{y}); \mathbf{b} = \sqrt{3}(\mathbf{x} + \mathbf{y}); \mathbf{c} = 2\mathbf{z}$.
What is the corresponding volume of the reciprocal space unit cell?

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

(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 $C_2 = ½\ C_1$. 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?

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

$$\omega^2 \approx \frac{4}{M}\left(C_1\frac{k^2a^2}{4} + C_2 k^2a^2\right) = \frac{4k^2a^2}{M}\left(\frac{C_1}{4} + \frac{C_1}{2}\right) = \frac{4k^2a^2C_1}{M}\frac{3}{4}$$

$$\omega = \sqrt{\frac{3k^2a^2C_1}{M}} = ka\sqrt{\frac{3C_1}{M}}$$

$$\underline{v_g = \frac{\partial\omega}{\partial k} = a\sqrt{\frac{3C_1}{M}}}$$

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?

<u>Answer: single crystal.</u>

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:

$\underline{k_1 = k_2 = 2\pi/3a}$ 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 spheroide-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 spheroide: $V_{sph} = \frac{4}{3}\pi r_a^{\,2} r_c$

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

Task 8-VI. Fermi pressure

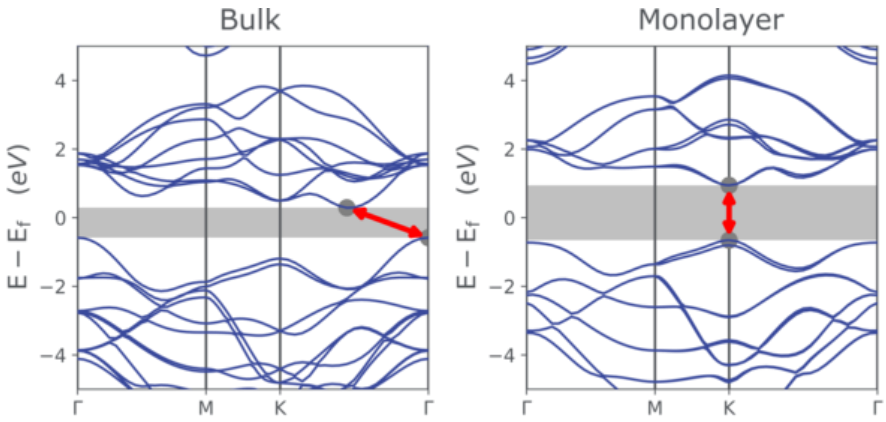
Thermodynamically, the pressure is related to the energy by $p = -\left.\frac{\partial U}{\partial V}\right)_{N\,const}$. One can thus derive that because of the volume dependence of the Fermi energy, $E_F \propto \left(\frac{N}{V}\right)^{2/3}$, the electron gas exerts a pressure.

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

Total energy of Fermi sphere ~ $E_0 + E_F \propto V^{-2/3}$, 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(. 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 $E_{tot} = \int_0^{E_F} ED(E)dE$.

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

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

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

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 **a** = a**x**, **b** = b**y** and **c** = *c* cos(β)**x** + *c* sin(β)**z**. The incoming X-ray beam is directed along **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 **X**,**Y**,**Z**, with **X** || **x**, **Y** || **y,** and **Z** || **z**.
Which expression gives a correct representation of the reciprocal lattice vector $\mathbf{G}_{100}$?

Answer:

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

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

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

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 **a** = a**x**, **b** = b**y** and **c** = *c* cos(β)**x** + *c* sin(β)**z**. The incoming X-ray beam is directed along **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 **X**,**Y**,**Z**, with **X** || **x**, **Y** || **y,** and **Z** || **z**.
Which expression gives a correct representation of the scattering vector **Q** that can be measured with the given geometry?

Answer:

$$\mathbf{k}_\mathbf{i} = \frac{2\pi}{\lambda}<0,1,0>,\ \mathbf{k}_f = \frac{2\pi}{\lambda}<0,\cos 2\theta,\sin 2\theta>$$

$$\mathbf{Q} \equiv \mathbf{k}_\mathbf{f} - \mathbf{k}_\mathbf{i} = \frac{2\pi}{\lambda}<0,\cos 2\theta - 1,\sin 2\theta>$$

Task 18. Inverse Umklapp

Version 1
In a rectangular 2D lattice with a = 6.90 Å and b = 4.50 Å, three phonons each having wave vector **k** = <0.80, 0.90> Å^{-1} merge to become one phonon. (Assume that the energy is conserved).

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

3**k** = <2.4, 2.7> Å^{-1}.
a = 6.90 Å → a^* = 2π/6.90 Å^{-1} = 0.91 Å^{-1}. 1st BZ boundary at 0.45 Å^{-1}.
b = 4.50 Å → b^* = 2π/4.50 Å^{-1} = 1.40 Å^{-1}. 1st BZ boundary at 0.70 Å^{-1}.

2.4 – 3·0.91 = -0.33
2.7 – 2·1.40 = -0.10
Answer: <-0.33, -0.10>

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

4**k** = <3.2, 3.6> Å^{-1}.
a = 6.90 Å → a^* = 2π/6.90 Å^{-1} = 0.91 Å^{-1}. 1st BZ boundary at 0.45 Å^{-1}.
b = 4.60 Å → b^* = 2π/4.60 Å^{-1} = 1.37 Å^{-1}. 1st BZ boundary at 0.68 Å^{-1}.

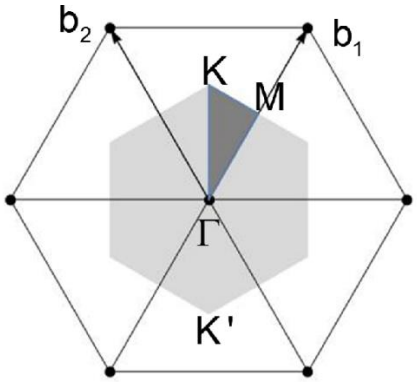
3.2 – 4·0.91 = -0.44
3.6 – 3·1.37 = -0.51
Answer: <-0.44, -0.51>

Version 3
In a rectangular 2D lattice with a = 6.90 Å and b = 4.60 Å, two phonons each having wave vector **k** = <0.80, 0.90> Å^{-1} merge to become one phonon. (Assume that the energy is conserved). What is the reduced zone scheme representation of the resulting phonon?

2**k** = <1.6, 1.8> Å^{-1}.
a = 6.90 Å → a^* = 2π/6.90 Å^{-1} = 0.91 Å^{-1}. 1st BZ boundary at 0.45 Å^{-1}.
b = 4.60 Å → b^* = 2π/4.60 Å^{-1} = 1.37 Å^{-1}. 1st BZ boundary at 0.68 Å^{-1}.

1.6 – 2·0.91 = -0.22
1.8 – 1·1.37 = 0.43
Answer: <-0.22, 0.43>

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

Answer:

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

With numbers: <u>E = 6.0 eV.</u>

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

<u>E = 3.0 eV</u>

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

<u>E = 8.0 eV</u>

(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

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

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

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

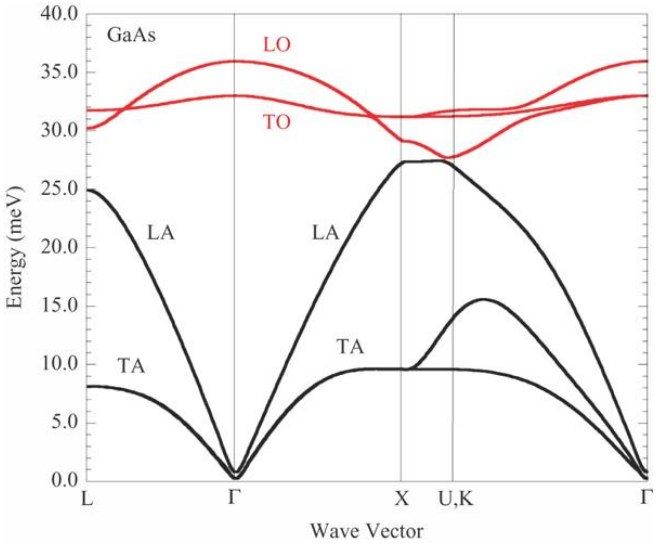
Task 20-IV. Bloch function

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



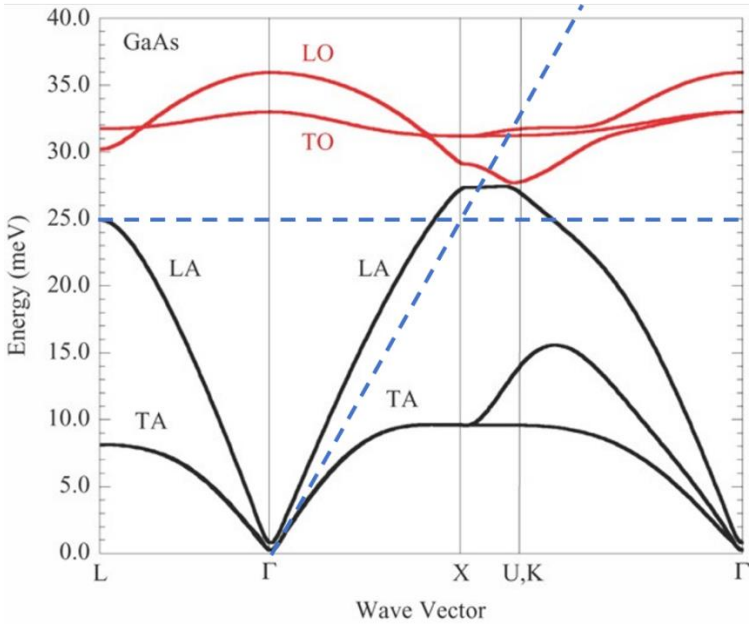
The figure shows the dispersion relations for lattice vibrations in GaAs, which is cubic with a = 5.65 Å. Find the approximate wavelength of the most strongly absorbed electromagnetic radiation by the LO phonons.

Answer:
Near the Γ point, the energy is E = 36.0 meV = 5.76e-21 J.

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

Thus, $\lambda=\frac{hc}{E}$ = <u>35 μm.</u>

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 Å. 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 meV.

Answer:
The energy at the intersection with the X point is 25 meV = 4.00e-21 J.
$\Delta\omega = E / \hbar$ = 3.79e13 rad^{-1}.
X-point: $\Delta k = 2\pi/a = 2$

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

25e-3*ee/hbar/(2*pi/5.65e-10) = 3410 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' = 12/5 $\pi^4 N k_B (T/T_D)^3$ Heat capacity for N atoms
C = $N_A \cdot C'/N$ = 12/5 $\pi^4 N k_B (T/T_D)^3$ Heat capacity for n moles

NA = 6.022e23;
kB = 1.38e-23;
C = 12*pi^4/5*kB*(180/1860)^3 * NA = 1.76 Answer: 1.7 J/(mol·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*kB*(160/1860)^3 * NA = 1.23 Answer: 1.2 J/(mol·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*kB*(140/1860)^3 * NA = 0.83 Answer: 0.8 J/(mol·K)