Front page

Department of Physics

Examination paper for TFY4220 Solid State Physics

Examination date: 20 May 2023

Examination time (from-to): 09:00 -13:00

Permitted examination support material:

Code C:
Approved calculator with empty memory.
K. Rottmann: Matematisk Formelsamling
S. Barnett & T.M. Cronin: Mathematical Formulae
O. Øgrim & B.E. Lian: Størrelser og enheter i fysikk og teknikk
C. Angell & B.E. Lian: Fysiske størrelser og enheter – navn og symboler

Academic contact during examination: Prof. Dag W. Breiby
Phone: 984 54213

Academic contact present at the exam location: No.

OTHER INFORMATION

Get an overview of the question set before you start answering the questions.

Read the questions carefully. Only contact academic contact in case of errors or insufficiencies in the question set. Address an invigilator if you wish to contact the academic contact. Write down the question in advance.

Weighting: This exam consists of 32 multiple choice tasks. Unless there are unexpected challenges, each task will be given equal weight during grading.

Notifications: If there is a need to send a message to the candidates during the exam (e.g. if there is an error in the question set), this will be done by sending a notification in Inspera. A dialogue box will appear. You can re-read the notification by clicking the bell icon in the top right-hand corner of the screen.

Withdrawing from the exam: If you become ill or wish to submit a blank test/withdraw from the exam for another reason, go to the menu in the top right-hand corner and click “Submit blank”. This cannot be undone, even if the test is still open.

Access to your answers: After the exam, you can find your answers in the archive in Inspera. Be aware that it may take a working day until any hand-written material is available in the archive.

1 **a.**

Which of these statements is *incorrect* regarding Bravais lattices?

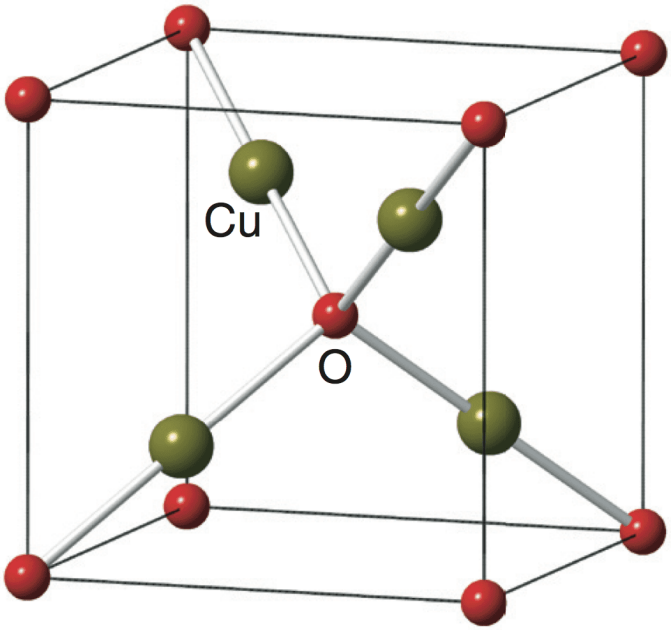
Select one alternative:

- The conventional unit cell of the face centered cubic Bravais lattice has angles α, β and γ all equal to 90°.
- A cubic unit cell with one Cs atom at each corner and another Cs atom in the center is simple cubic. ✔
- A Bravais lattice consists of all points with position vector **R** of the form $\mathbf{R} = n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3$, where $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ are any three vectors not all in the same plane, and n_1, n_2, n_3 range through all integer values.
- The only possibilities for cubic Bravais lattices are simple cubic, face centered cubic and body centered cubic.
- A Bravais lattice is an infinite array of discrete points with an arrangement and orientation that appears exactly the same, from whichever of the points the lattice is viewed.

Maximum marks: 1

2 a)

Cuprite has a unit cell as shown in the figure:



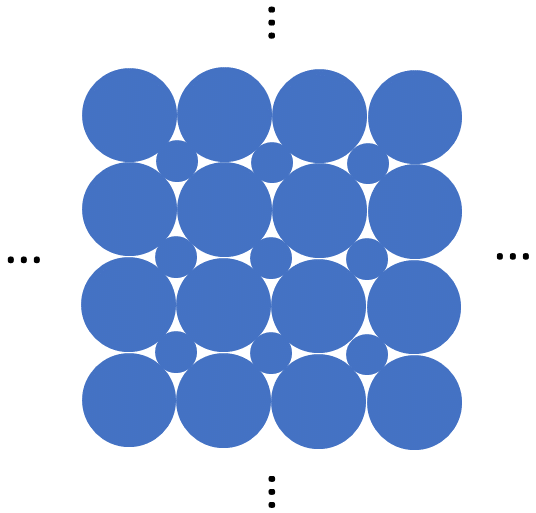
The unit cell is cubic, and the Cu atoms are located midway between the oxygen atoms at the center and at the corners.
Which of the following is a valid description of the relative coordinates of the basis?

Select one alternative:

- *O*: (0,0,0), (0.5, 0.5, 0.5), (1,0,0), (0,1,0), (1,1,0), (0,0,1), (1,0,1), (0,1,1), (1,1,1)
  Cu: (0.25, 0.25, 0.25), (0.75, 0.75, 0.25), (0.25, 0.25, 0.75), (0.75, 0.25, 0.75)
- *O*: (0,0,0), (0.5, 0.5, 0.5)
  Cu: (0.25, 0.25, 0.25), (0.75, 0.75, 0.25), (0.25, 0.25, 0.75), (0.75, 0.75, 0.75)
- *O*: (1,1,1), (1.5, 1.5, 1.5)
  Cu: (0.25, 0.25, 0.25), (0.75, 0.75, 0.25), (0.25, 0.75, 0.75), (0.75, 0.25, 0.75) ✔
- *O*: (0.5,0.5,0.5)
  Cu: (0.25, 0.25, 0.25); (0.25, 0.75, 0.75)
- *O*: (0,0,0), (0.5, 0.5, 0.5)
  Cu: (0.25, 0.25, 0.25), (0.75, 0.75, 0.25), (0.25, 0.25, 0.75), (0.75, 0.25, 0.75)

Maximum marks: 1

3 **a:.**



The shown dense 2D packing consists of circular disks of two different diameters in close contact, with the ratio of their radii allowing the small disks to fit exactly into the voids between the larger disks. (Consider the pattern to extend laterally to +/- infinity, as indicated by the dots).

What is the planar group of the 2D structure shown?

Select one alternative:

- Centred rectangular
- Oblique
- Rectangular
- Square ✔
- Hexagonal

Maximum marks: 1

4 a):

For a hexagonal unit cell, the lattice spacing is given by

$$\frac{1}{d_{hkl}^2} = \frac{4}{3}\frac{h^2+hk+k^2}{a^2} + \frac{l^2}{c^2}.$$

In a powder X-ray diffraction experiment using a monochromatized beam, the $2\bar{1}0$ diffraction ring was seen to overlap with the diffraction ring of the 001 peak. What is the ratio of the unit cell lengths a/c for this overlap to occur?

Select one alternative:

- $a/c = 1/\sqrt{3}$
- $a/c = 3$
- $a/c = \sqrt{2}$
- $a/c = 5$
- $a/c = 2$ ✔

Maximum marks: 1

5 a).

In a powder diffraction experiment, high-energy X-rays with photon energy E = 80.0 keV are used. A Bragg diffraction peak is observed at a scattering angle 2θ = 28.7°.

What is the corresponding layer spacing d?

Select one alternative:

- d = 3.11 Å
- d = 0.31 Å ✔
- Cannot be answered because the sample orientation is not specified.
- d = 3.11 $Å^{-1}$
- d = 1.61 Å

Maximum marks: 1

6 a)::

Copper is fcc and has a lattice constant of a = 361.49 pm.
What is the shortest distance between nearest-neighbor atomic centers in a copper crystal? (ignore temporal variations like phonons).

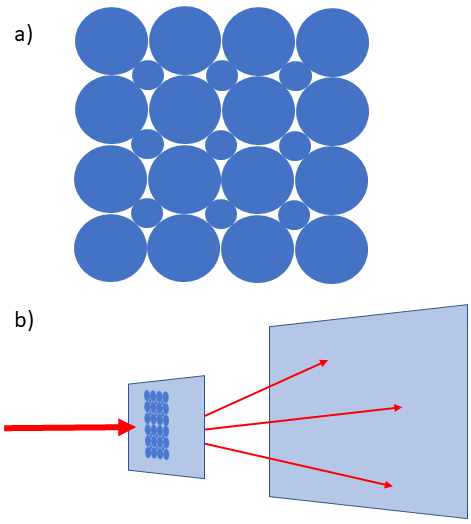
Select one alternative:

- 2.56 Å ✔
- 3.61 Å
- 1.80 Å
- 3.13 Å
- 5.11 Å

Maximum marks: 1

7 a::

The shown dense 2D packing consists of circular disks of two different diameters in close contact, with the ratio of their radii allowing the small disks to fit exactly into the void between the larger disks, see Fig. a). This pattern is used as a micrometer-scale 2D semi-transparent object in a laser diffraction experiment (as illustrated in Fig. b), where the dense packed disks impose a phase shift and/or an attenuation of the light wave front.



Which statement is correct regarding the Fraunhofer diffraction pattern?
(*F* denotes the Fourier transform; ρ the density distribution).

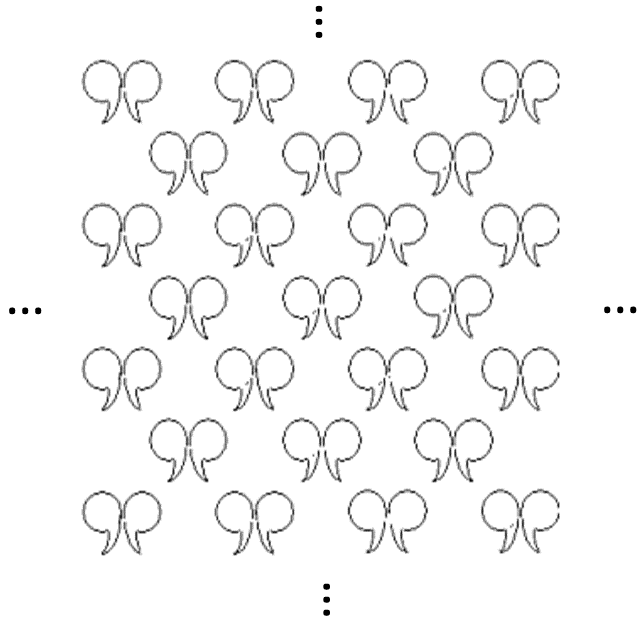
Select one alternative:

- The diffraction pattern will not contain information about the relative diameters of the disks.
- The amplitude distribution can be described by $A \sim F\{\rho(x,y)\}$. ✔
- The diffraction pattern will exhibit 6-fold symmetry.
- The intensity can be described by $I \sim |F\{\rho(x,y)\}|^{1/2}$.
- The **Q** = **G** diffraction condition does not apply to this setup.

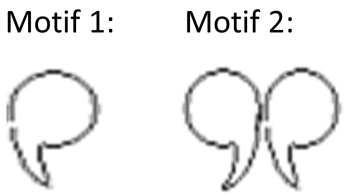
Maximum marks: 1

8 a:

A repeated pattern is shown in the figure below.



(Consider the pattern to extend laterally to +/- infinity, as indicated by the dots)
For the alternatives, the following motifs are needed:



Which of the statements is *correct* regarding the repeated pattern given above?

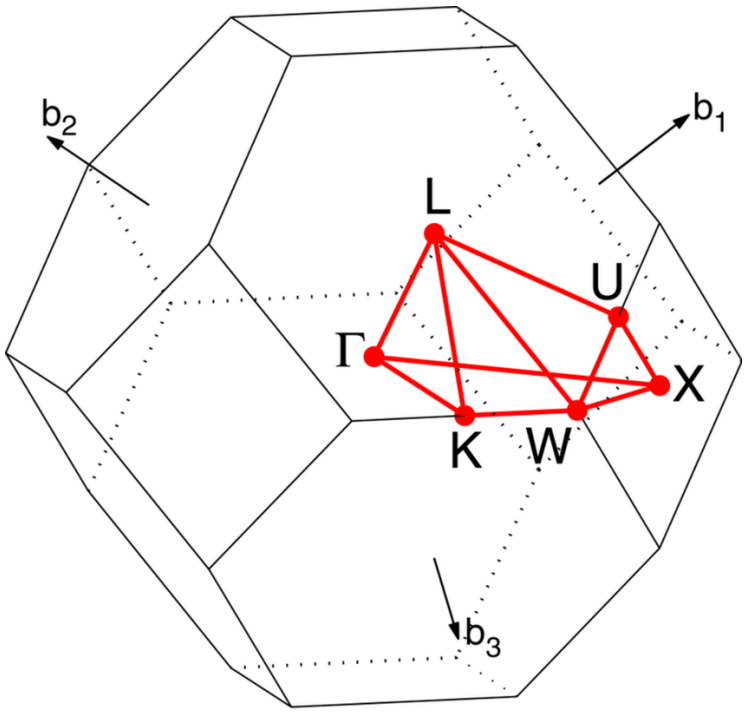
Select one alternative:

- The pattern has two-fold symmetry.
- The pattern can be described as a Bravais lattice convoluted with the basis *Motif 1*.
- The pattern can be described as a convolution between a (2D) square lattice and *M* ✔ 2.
- The pattern is a Bravais lattice.
- The pattern has vertical and diagonal mirror planes.

Maximum marks: 1

9 a):.

A central figure from the lectures is reproduced in the image below:



Which statement is correct?

Select one alternative:

- The figure shows the first Brillouin zone of a simple cubic Bravais lattice.
- The figure shows the first Brillouin zone of a face-centered cubic Bravais lattice. ✔
- The points Γ, K, L, U, X, W are all at the Brillouin zone boundary.
- The X-point is at the origin of reciprocal space.
- The red lines describe all the directions that can be defined in reciprocal space.

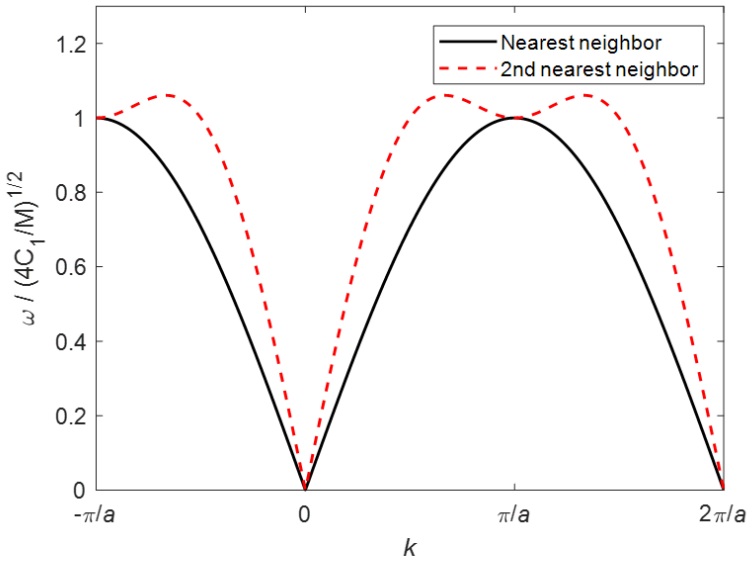
Maximum marks: 1

10 **b.**

It can be shown that the dispersion relation $\omega(k)$ for phonons on a 1D string with interactions between next-nearest neighbors included is given by

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

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.
The dispersion relation is plotted in the figure (red broken line), assuming C_2 = ½ C_1. For comparison, the standard nearest-neighbor dispersion relation with the same values for C_1 and M is also given (black line).



Which of the following statements is *incorrect* for this phonon model including 2nd nearest neighbors interactions, as shown in the graph?

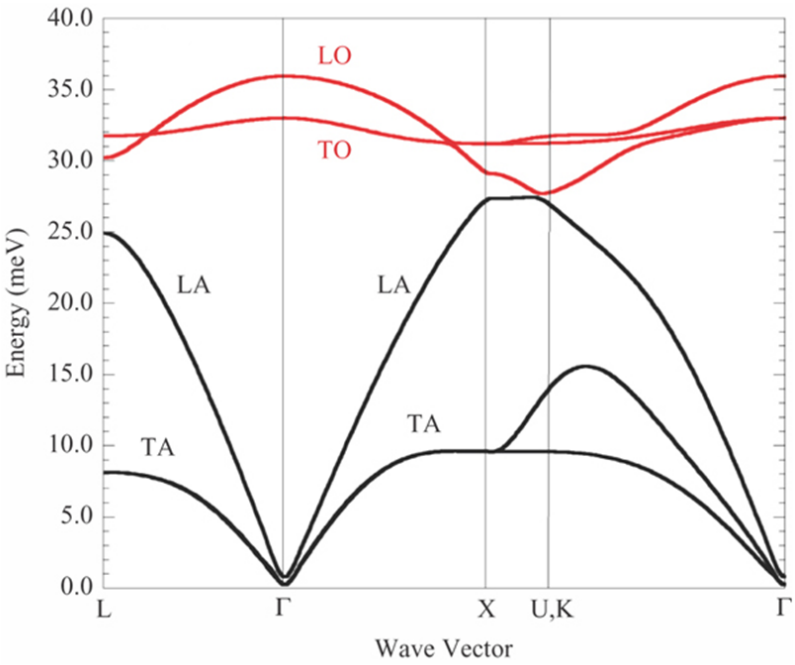
Select one alternative:

- The density of states diverges also at points with $|k| \neq \frac{\pi}{a}$.
- The density of states at small k is higher when including the 2nd nearest neighbor interactions. ✔
- The density of states diverges at the BZ boundary for both models.
- A qualitatively new feature is that there is now a region in k-space where the signs of v_{phase} and v_{group} differ.
- The maximum frequency has increased when including the 2nd nearest neighbor interactions.

Maximum marks: 1

11 b:.

The phonon spectrum for a 3D material is shown in the figure.



How many atoms are there in the primitive unit cell?

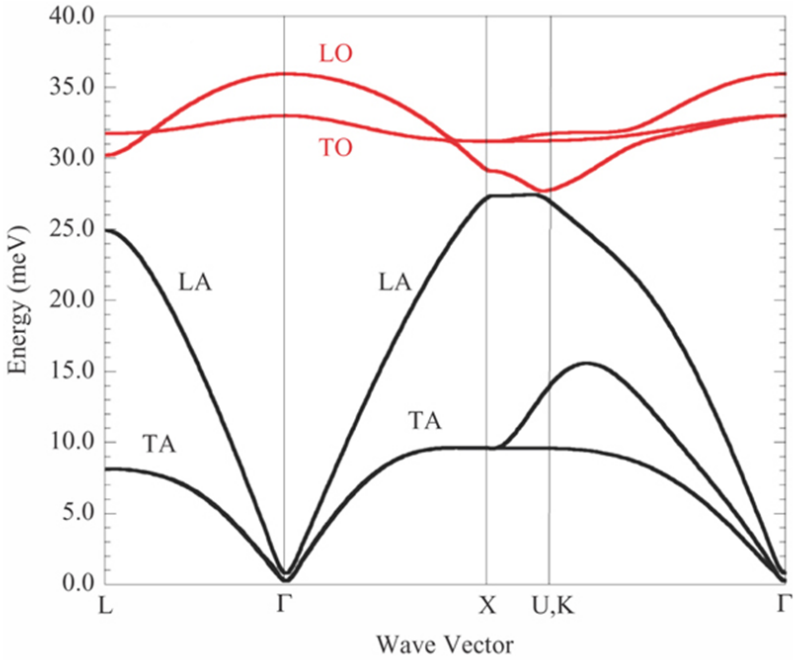
Select one alternative:

- > 2
- 6
- 3
- 2 ✔
- 1

Maximum marks: 1

12 b::

The phonon spectrum for a 3D solid material is shown in the figure.



Which statement is correct?

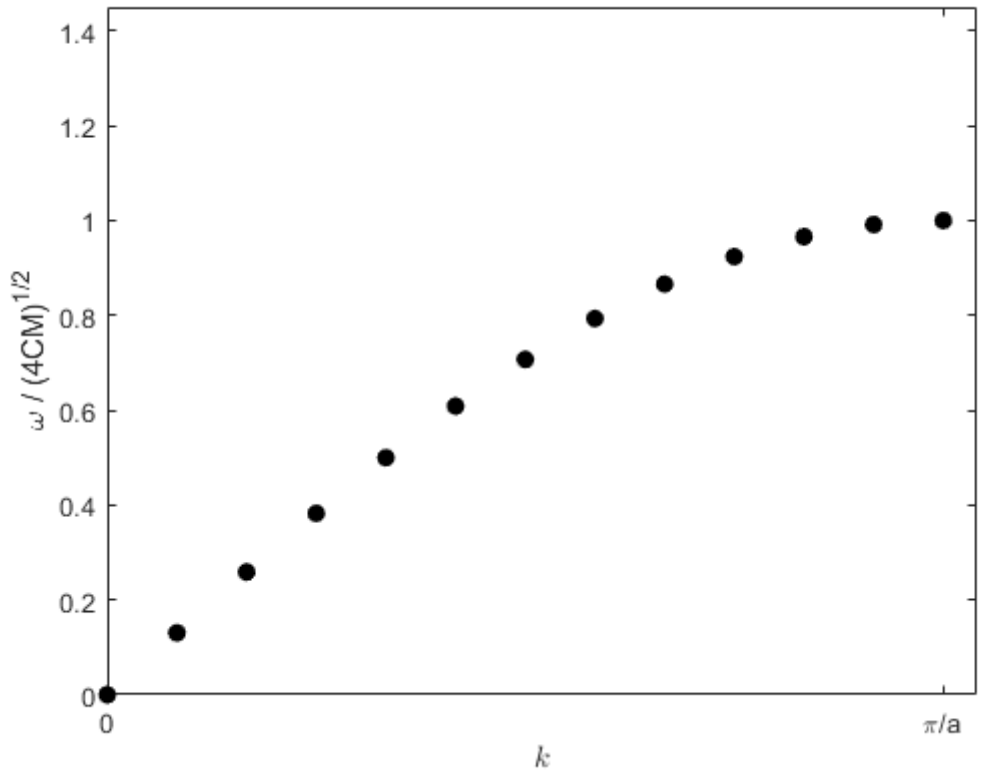
Select one alternative:

- The degeneracy is usually independent of the crystal symmetry.
- The longitudinal sound waves travel significantly more slowly than the transversal sound waves.
- The TA modes along the $\Gamma - X$ path are degenerate. ✔
- There is no degeneracy.
- The optical modes are inversely degenerate at Γ and at X.

Maximum marks: 1

13 **b).**

The phonon dispersion relation for a nanoscale 1D linear monoatomic linear chain is plotted for $k \in (0, \pi/a)$ in the figure below:



The dots mark the discrete *k*-values consistent with the finite lattice.
How many atoms long is the string?

Select one alternative:

- of the order of 10^{23}
- 13
- 2
- 24 ✔
- 1

Maximum marks: 1

14 **b:**

Given facts:
- Iron is bcc with one atom in the basis
- MnO is fcc (halite / "rock salt" structure) with two atoms in the basis

Which of the following statements about phonons is *incorrect*?

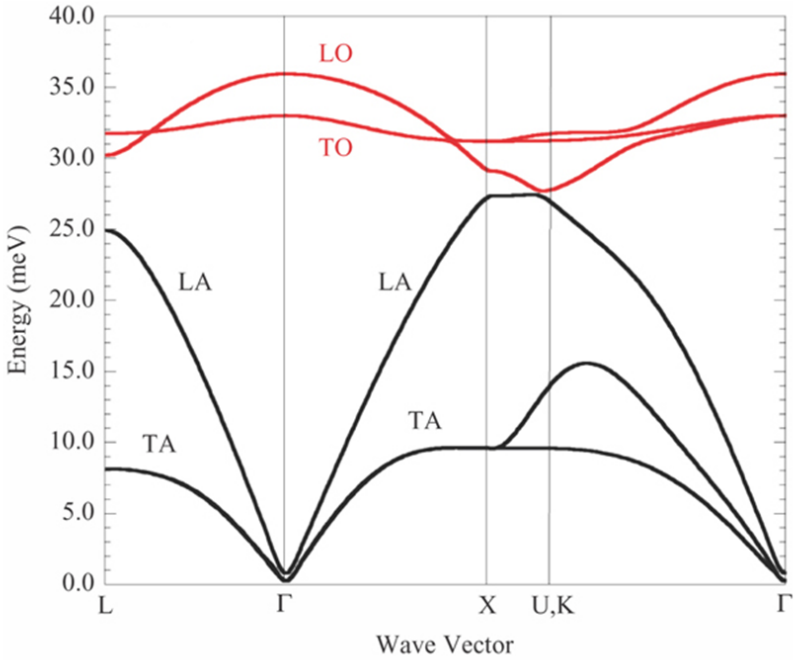
Select one alternative:

- Iron has acoustic and optical phonons because there are two atoms in the conventional unit cell. ✔
- The Einstein model predicts that the heat capacity C goes to zero when T approaches zero.
- MnO has acoustic and optical phonons because there are two atoms in the primitive unit cell.
- For a 1D linear chain, the number of possible values of k equals $\log(N)$, where N is the number of unit cells.
- The equipartition theorem predicts that the phonon heat capacity is constant for all T.

Maximum marks: 1

15 **b)**

The phonon spectrum for a 3D material is shown in the figure.



Consider a two-particle process where an incoming photon is absorbed and a phonon created. What is the photon wavelength that will give a high probability for such a two-particle process to take place with the transverse phonons?

Select one alternative:

- 1.54 Å
- 14 μm
- 42 μm
- 532 nm
- 38 μm ✔

Maximum marks: 1

16 **c):.**

A translation operator $\hat{T}_R$ has the property that
$\hat{T}_R\psi(\mathbf{r}) = \psi(\mathbf{r}+\mathbf{R})$, where $\mathbf{R}$ is a lattice translation vector and $\psi(\mathbf{r})$ is a wave function.
Let the translation operator act on a Bloch state $\psi_k(\mathbf{r})$.
Which expression is correct for the eigenvalue of $\hat{T}_R\psi_k(\mathbf{r})$?

Select one alternative:

- $\exp(i\mathbf{G}\cdot\mathbf{r})$
- $\exp(i\mathbf{k}\cdot\mathbf{R})$ ✔
- $\exp(i\mathbf{G}\cdot\mathbf{R}) = 1$
- The eigenvalue does not exist.
- $\exp(i\mathbf{k}\cdot\mathbf{r})$

Maximum marks: 1

17 **c:.**

An element has a face-centered cubic unit cell with *a* = 0.409 nm. There is one atom in the basis. Assuming that each atom gives 1 electron to conduction, estimate the Fermi temperature of this element.

Given:
$E_F = \frac{\hbar^2}{2m_e}\left(\frac{3\pi^2 N}{V}\right)^{2/3}$

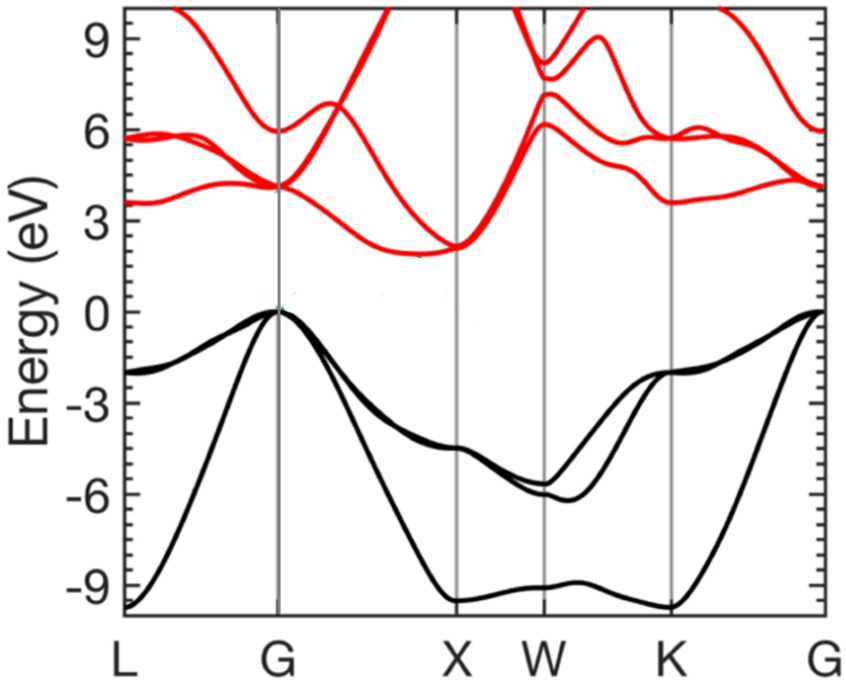
Select one alternative:

- 60 000 K
- 56 000 K
- 0 K
- approx. 10^6 K
- 64 000 K ✔

Maximum marks: 1

18 **c.**

The electronic structure of a diatomic compound is shown in the figure:



Energy = 0 defines the highest-energy occupied electron states at T = 0 K. G denotes the Gamma point.

Which kind of material is this?

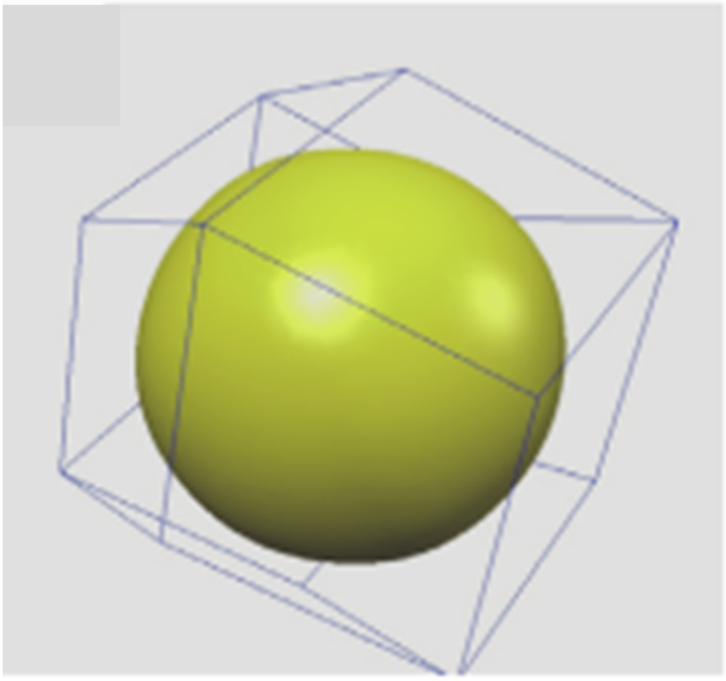
Select one alternative:

- An insulator
- An indirect bandgap semiconductor ✔
- A direct bandgap semiconductor
- A metal
- A semimetal

Maximum marks: 1

19 **c).**

The figure below shows an experimentally measured Fermi surface for a metal, contained within the 1st Brillouin zone.



Which of the following statements is *correct?*

Select one alternative:

- When deriving the free electron Fermi gas model, it is assumed that the potential has half the periodicity of the lattice.
- The Fermi surface shown in the figure suggests that the free electron Fermi gas is a good model for this material.
- The volume of the Fermi sphere at $T = 0$ can be expressed as $\left(\frac{2\pi N}{L}\right)^3 \cdot \frac{1}{2}$, where N is the number of primitive unit cells and L^3 is the volume of the crystal.
- The free electron Fermi gas model can account for the electronic contributions to the heat capacity, $C_{el} \propto T^3$ at low T.
- The free electron Fermi gas model predicts that in k-space, the electrons arrange in a Fermi sphere of radius $k_F/2$ at $T = 0$.

Maximum marks: 1

20 **c)::**

If the quantum mechanical momentum operator $\hat{\mathbf{p}} = -i\hbar\nabla$ is applied to a Bloch state $\psi_{\boldsymbol{k}}$, what is the corresponding eigenvalue?

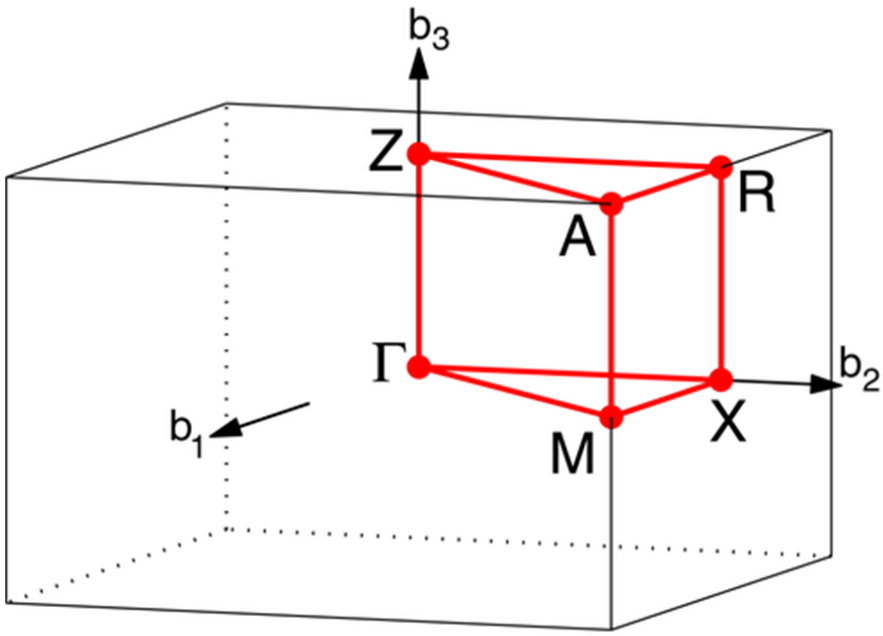
Select one alternative:

- $\exp(i\mathbf{k}\cdot\mathbf{r})$
- 1
- 0
- $\hbar\mathbf{k}$
- The eigenvalue does not exist ✔

Maximum marks: 1

21 **c:**

The R-point for a simple tetragonal lattice ($a_1 = a_2 \neq a_3$, all angles 90°) is defined in the figure below.



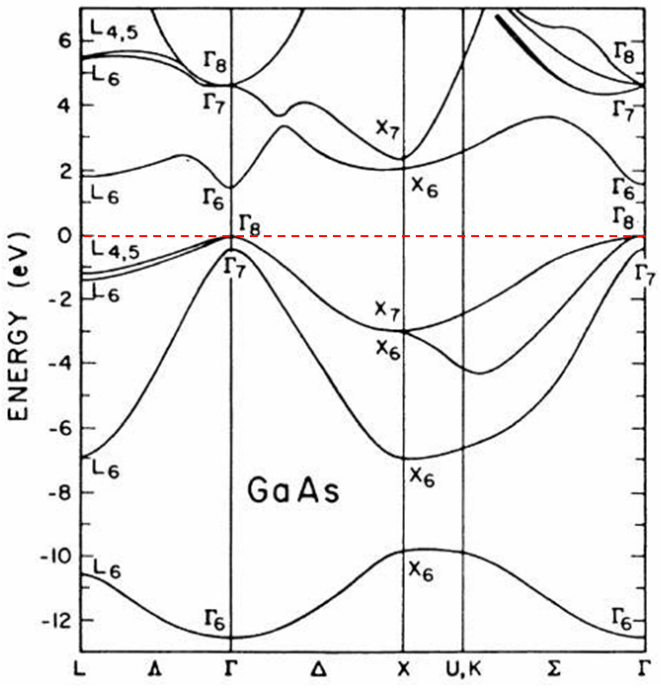
What is the energy of an electron at the R-point according to the "free electron Fermi gas" model? Define the energy at the Γ-point to be zero.

Select one alternative:

- $E_R = \frac{\pi^2\hbar^2}{2m}\left(\frac{1}{a_1^2} + \frac{1}{a_3^2}\right)$ ✔
- $E_R = \frac{2\pi^2\hbar^2}{m}\frac{1}{a_2}\sqrt{\frac{1}{a_1^2} + \frac{1}{a_3^2}}$
- $E_R = 0$
- $E_R = \frac{\hbar^2 k^2}{2m}\frac{1}{a_1 a_3}$
- $E_R = \frac{\pi^2\hbar^2}{m a_1^2}$

Maximum marks: 1

22 **c)**



The above figure shows the band structure of intrinsic GaAs. The broken red line indicates the top of the valence band (with energy defined to be zero).

Which one of the following statements is *incorrect*?

Select one alternative:

- Γ_8 is the most probable state to be vacated after electronic excitation to the conduction band.
- At room temperature, there will be no holes at Γ_8. ✔
- The material has a direct bandgap.
- The point Γ_8 is at an energy maximum of a hole band, corresponding to hole states with $m_h > 0$.
- At $T = 0$ K, electrons at Γ_8 will be moving with a speed of the order of 10^3 km/s.

Maximum marks: 1

23 **c):**

Which of the following statements is *incorrect* regarding the Fermi sphere?

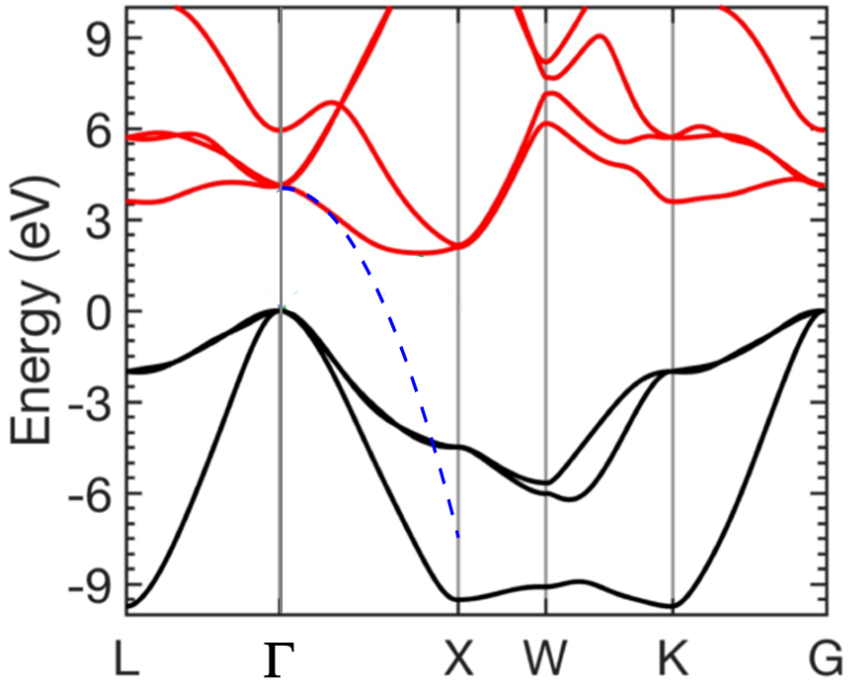
Select one alternative:

- If the size of the crystal is doubled along one or more dimensions, the Fermi sphere stays the same.
- The electrons residing near the surface of the Fermi sphere are not moving in reciprocal space at $T = 0$ K.
- Only electrons near the Fermi level can be thermally excited to higher energy levels at room temperature.
- Only electrons near the surface of the Fermi sphere shifts in k if an electric field is applied across the specimen. ✔
- The Fermi wave vector k_F is of the order of 10^9 m^{-1}.

Maximum marks: 1

24 **c::**

The electronic band structure of a compound having the zinc blende structure (fcc) with *a* = 4.78 Å is given below.



The blue broken line is a parabola fitted to the lowest-energy conduction branch near the Γ-point along the ΓX-path. The energy is defined to be zero at the top of the valence band. The direct bandgap at Γ is 4.1 eV. For fcc structures, the X-point is at $2\pi/a$.

The fitted parabola intersects the Brillouin zone at the X-point with an energy of -7.9 eV.
For the fitted band, what is the approximate effective electron mass near the Γ-point ?

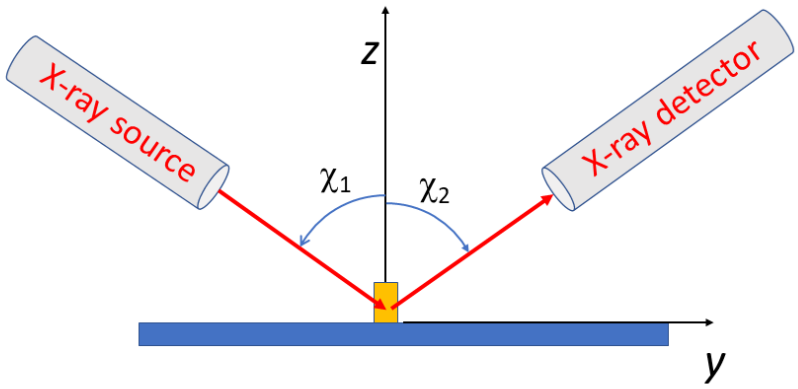
Select one alternative:

- 0.55 m_e
- -1.05 m_e
- -0.95 m_e
- 0.95 m_e
- -0.55 m_e ✔

Maximum marks: 1

25 **d.**

A single crystal is fixed in an orthogonal laboratory coordinate system $(\mathbf{x}, \mathbf{y}, \mathbf{z})$, where $\mathbf{z}$ is the vertical direction. The crystal belongs to the orthorhombic crystal system and is oriented with the unit cell *c*-axis parallel to the laboratory *z*-axis. The incoming monochromatic X-ray beam is in the $(\mathbf{y}, \mathbf{z})$ plane, with an incidence angle χ_1 with respect to the *z*-axis as shown in the figure. The point detector (sensor) is placed in the $(\mathbf{y}, \mathbf{z})$ plane, and is oriented to accept scattered radiation having an angle χ_2 with respect to the *z*-axis, as shown in the figure.
Note: the sketch is not to scale, the small crystal sample is assumed to be flooded (fully covered) by the X-ray beam.



The experimenter wants to measure the diffracted intensity from the *001* Bragg peak.
Which of the statements is correct?

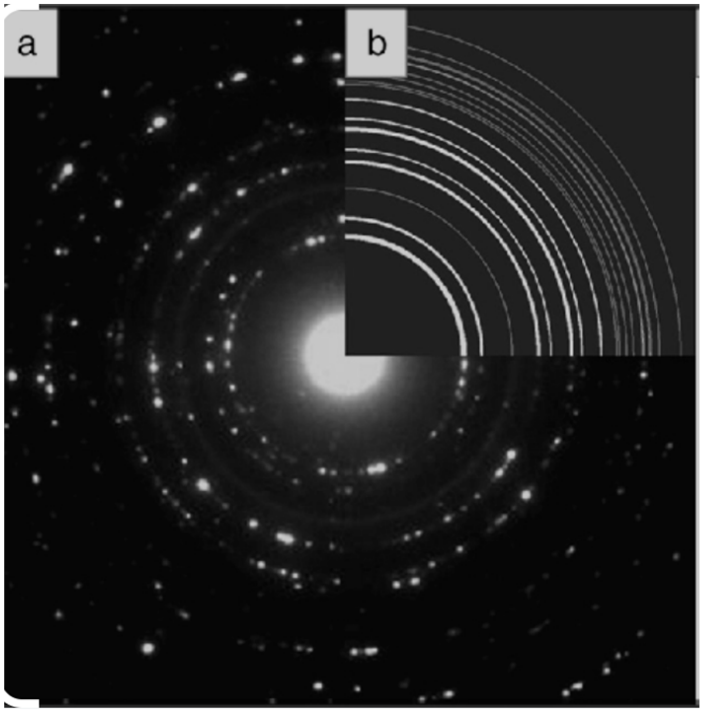
Select one alternative:

- If $\chi_1 = \chi_2$, the scattering vector **Q** will be directed along the *x*-axis.
- If χ_2 = 90°, the scattering vector **Q** will be directed along the *y*-axis.
- With the given orientation of the sample, a sufficient requirement for the diffraction condition **Q** = $\mathbf{G}_{001}$ to be fulfilled is that χ_1 = χ_2.
- The scattering angle is given by $2\theta = 360^o - (\chi_1 + \chi_2)$.
- If the diffraction condition **Q** = $\mathbf{G}_{001}$ is fulfilled with χ_1= χ_2, the scattered intensity will be constant (within experimental error) if the sample is being rotated about the **z**-axis. ✔

Maximum marks: 1

26 d:

Using selected area electron diffraction (SAED), the following diffraction patterns a) and b) have been recorded for the same compound:



Which statements are correct?

Select one alternative:

- The sample in a) is polycrystalline; the sample in b) is a nearly ideal powder. ✔
- The sample in a) is polycrystalline; the sample in b) is amorphous.
- Both patterns are consistent with amorphous samples.
- The sample in a) is amorphous; the sample in b) is a nearly ideal crystalline powder.
- The sample in a) is a single crystal; the sample in b) is a nearly ideal powder.

Maximum marks: 1

27 **d:.**

Which structure has the highest packing fraction?

Select one alternative:

- Diamond structure
- Hexagonal close packed ✔
- Body centered cubic
- Simple cubic
- Monoclinic

Maximum marks: 1

28 **d::**

At small wave vector k, the group velocity and phase velocity coincide for which one of the following categories of phonon modes?

Select one alternative:

- Acoustic ✔
- Optical
- Longitudinal (both LO and LA)
- Transverse (both TO and TA)
- Acoustic and optical

Maximum marks: 1

29 **d)**

A linear monoatomic lattice in 1D has dispersion relation

$$\omega = \sqrt{\frac{4C}{M}} \left| \sin \frac{ka}{2} \right|,$$

which has a maximum frequency ω_{max} at $k = \pm\pi/a$.
If the crystal is forced into an oscillation mode with $\omega > \omega_{max}$, what will happen?

Select one alternative:

- The phonon will be imaginary, and thus not observable.
- The wave will get damped exponentially with distance; the oscillation mode cannot be sustained in the lattice. ✔
- The heat capacity will increase.
- The crystal will get unstable and eventually disintegrate because of anharmonic effects.
- A global phase factor without physical consequences will be multiplied into the wave function.

Maximum marks: 1

30 **d).**

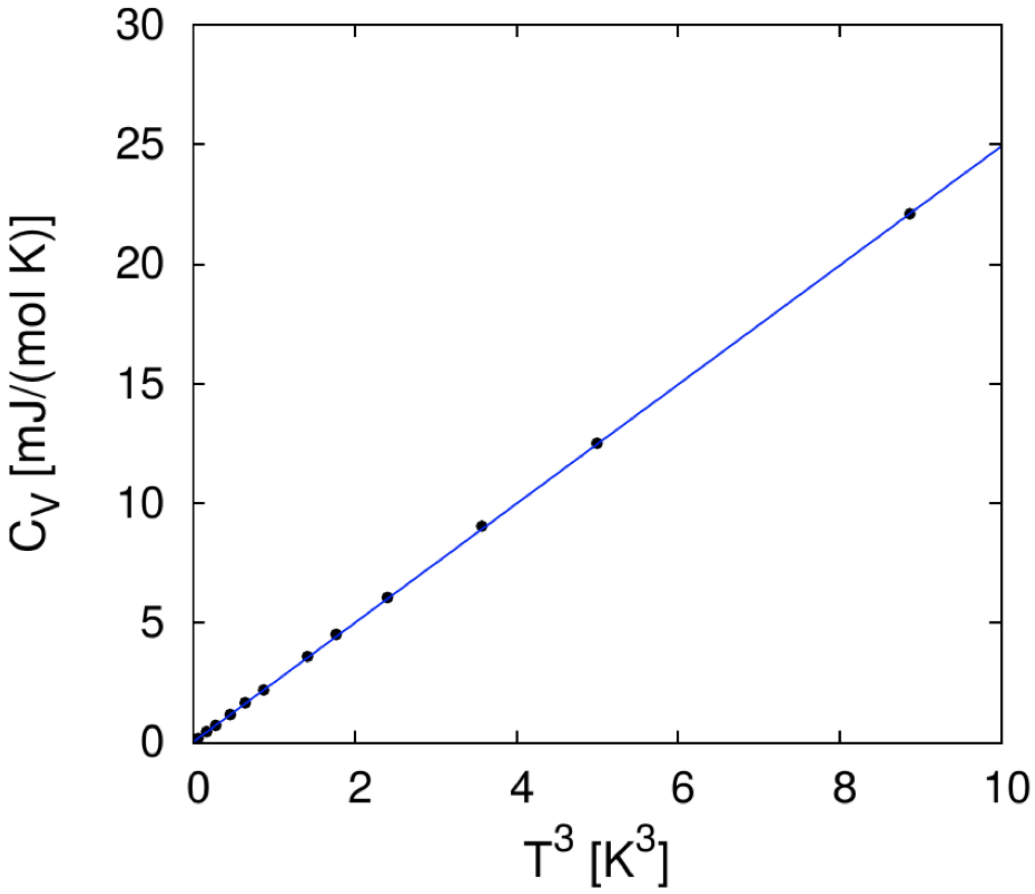
Which statement is true regarding the electrical conductivity of materials?
Select one alternative:

- The electrical conductivity of a metal increases with increasing temperature.
- The electrical conductivity of a metal decreases with increasing temperature. ✔
- The electrical conductivity of a semiconductor is temperature independent.
- The electrical conductivity of a semiconductor decreases with increasing temperature.
- The electrical conductivity of a metal is proportional to T^{-3} at all temperatures.

Maximum marks: 1

31 **d):**

In the low temperature limit, the Debye T^3 law can be expressed as
$C_V \approx 234 N k_B (\frac{T^3}{\theta^3})$.
The figure shows experimental calorimetric data for a solid material, with the heat capacity plotted as a function of T^3.



Use the provided graph with experimental data to estimate the Debye temperature θ for this material. What is the Debye temperature?

Select one alternative:

- 92 K ✔
- 102 K
- 920 K
- 273 K
- 0 K

Maximum marks: 1

32 **d):.**

What is the Fermi velocity v_F for lead (Pb)? For Pb, $E_F = 9.37$ eV.

Select one alternative:

- 9.9×10^5 m/s
- 1.8×10^6 m/s ✔
- 8.7×10^6 m/s
- $v_F = c$ (the speed of light)
- 0, the Fermi speed at the Brillouin zone boundary must be zero.

Maximum marks: 1