Exam TFY4220 Spring 2019

NTNU

Department of Physics

Examination paper for TFY4220 Solid State Physics

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Examination date: 6 June 2019
Examination time (from-to): 0900 - 1300
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

Other information: None.

Language: English

2 p per correct answer.
No points for notes.

1

MC 1.1

Condensed matter physics largely considers physical processes over what range of energies?
Select one alternative:

- μeV to eV
- meV to keV
- keV to MeV
- MeV to GeV
- all of the above

Maximum marks: 2

2

MC 1.2

What is the approximate distance between atoms in a copper crystal?
Select one alternative:

- 0.3 Å
- 30 Å
- 0.3 nm
- 30 nm
- 3 μm

Maximum marks: 2

3

MC 1.3

The number of different 3D Bravais lattices is

Select one alternative:

- 3
- 14
- 167
- $2\pi/a$ where *a* is the lattice spacing.
- unlimited

Maximum marks: 2

4

MC 1.4

In its cubic unit cell, $BaTiO_3$ (barium titanate) has barium atoms positioned at the 8 cell corners, a titanium atom in the middle, and oxygen atoms centred at each of the 6 faces. What is the number of atoms in the crystal basis?

Select one alternative:

- 3
- 4
- 5
- 8
- 15

Maximum marks: 2

5

MC 1.5

Which structure has the highest packing fraction?

Select one alternative:

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

Maximum marks: 2

6

MC 1.6

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: 2

7

MC 1.7

If a crystal with two atoms per primitive basis is forced into an oscillation mode in the forbidden frequency region, it can be shown that the corresponding wave vector k gets complex. What consequence does the complex k have?

Select one alternative:

- The wave gets exponentially damped and dies out over a short distance.
- The phonon will be imaginary, and thus not observable.
- The crystal gets unstable because of anharmonic effects.
- The heat capacity will increase.
- No consequence, just a global phase factor without physical consequences

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Maximum marks: 2

8

MC 1.8

Which statement is true regarding the electrical conductivity of materials?

Select one alternative:

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

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Maximum marks: 2

9

MC 1.9

For metals the conduction band and valence band are

Select one alternative:

- Fully degenerate
- Empty
- Fully occupied
- Overlapping
- The valence band is empty, the conduction band is full.

Maximum marks: 2

10

MC 1.10

The electron and hole concentrations in an intrinsic semiconductor are n_i and p_i, respectively. When doped to a p-type material, these change to n and p, respectively. Then:

Select one alternative:

- $np = n_i p_i$
- $n + n_i = p + p_i$
- $n = p$
- $n + p = n_i + p_i$
- None of the above

Maximum marks: 2

11

MC 1.11

The Fermi level represents an energy level with probability of occupation equal to

Select one alternative:

- 0 %
- 25 %
- 50 %
- 100 %
- The answer depends on the crystal structure

Maximum marks: 2

12

MC 1.12

What is the Fermi speed u_F for gold (Au)? Remember that u_F is the speed of a conduction electron whose energy is equal to the Fermi energy E_F. For Au, $E_F = 5.55$ eV.

Select one alternative:

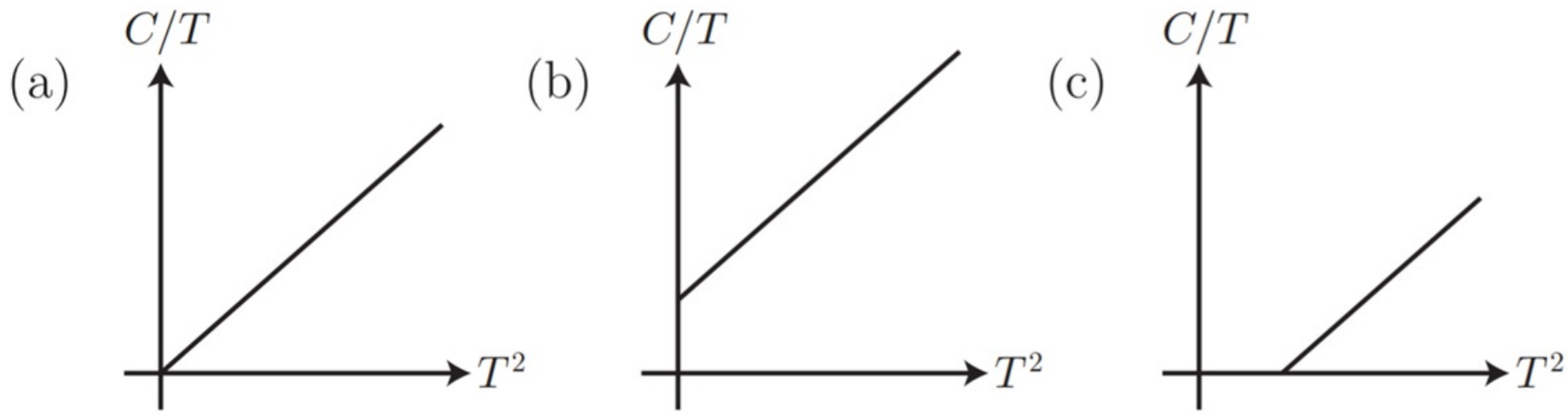
- 9.9×10^5 m/s
- 1.4×10^6 m/s
- 8.7×10^{24} m/s
- $u_F = c$ (the speed of light)
- 0, the Fermi speed at the Brillouin zone boundary must be zero.

Maximum marks: 2

13

MC 1.13

The total heat capacity of a material is the sum $C = C_{el} + C_{ph}$ of its electron and phonon contributions. Which of the following graphs describes a metal at low T?



Select one alternative

- Fig. (a)
- Fig. (b)
- Fig. (c)
- All of the figures, depending on the impurity levels.
- None of these figures.

Maximum marks: 2

14

MC 1.14

Free electrons with wavefunction $\psi \sim \exp(i\mathbf{k}\cdot\mathbf{r})$ are characterized by a quantum number $\mathbf{k} = (k_x, k_y, k_z)$ and have energy $E(\mathbf{k}) = \hbar^2|\mathbf{k}|^2/2\mathbf{m}$

Which of the following correctly describes the ground state of N electrons in a volume V with Fermi energy $E_F = (\hbar^2/2m)(3\pi^2 N/V)^{2/3}$?

Select one alternative:

- all states with $(k_x^2 + k_y^2 + k_z^2)^{1/2} > (3\pi^2 N/V)^{1/3}$ are filled
- all states with $(k_x^2 + k_y^2 + k_z^2)^{1/2} < (3\pi^2 N/V)^{1/3}$ are filled
- All the electrons will be in the ground state (with $E = 0$)
- all states with $-E_F/2 < E(\mathbf{k}) < E_F/2$ are filled
- The answer cannot be answered because the spin states are not specified.

Maximum marks: 2

15

MC 1.15

A diatomic gas is held at room temperature. Which of the following excitation modes is NOT significantly occupied?

Select one alternative:

- vibrational
- electronic
- rotational, vibrational and electronic
- vibrational and electronic
- rotational

Maximum marks: 2

Short text problems.
Only the digital form should be used.
The maximal number of points is indicated for each problem.

16

2.1 About X-rays (5 points)

- What energy (in units of eV) and corresponding wavelength (in units of nm) must X-ray photons have if they are to be used in diffraction experiments with the purpose of characterizing crystal structure?
- When X-rays scatter from a material, how do they interact with the atoms?

Fill in your answer here

Format

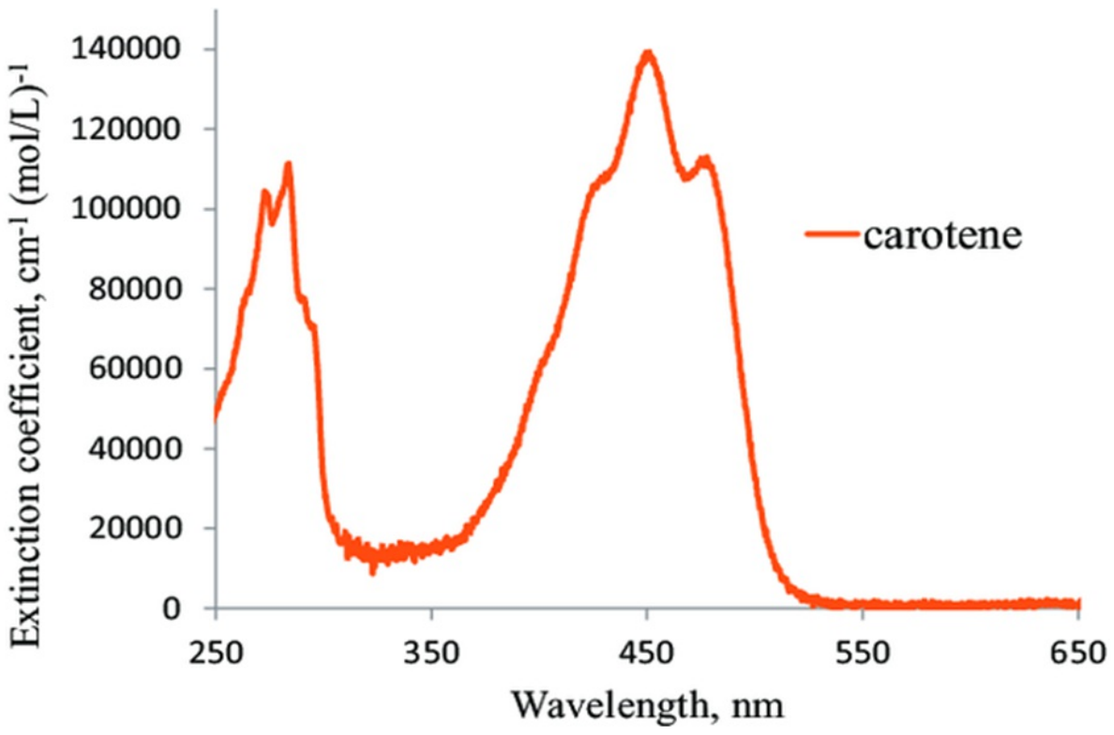
Words: 0

Maximum marks: 5

17

2.2 Beta-carotene (10 points)

Beta-carotene, a molecule abundant in carrots, has a UV-vis absorption spectrum as shown above.



- Explain shortly how a spectrum like this is obtained!
- Explain why this spectrum is consistent with beta-carotene being a semiconductor!
- What is the energy (in units of eV) of the bandgap?

Fill in your answer here

Format | B I U x_2 x^2 I_x | Ω | ∑ | ABC

Words: 0

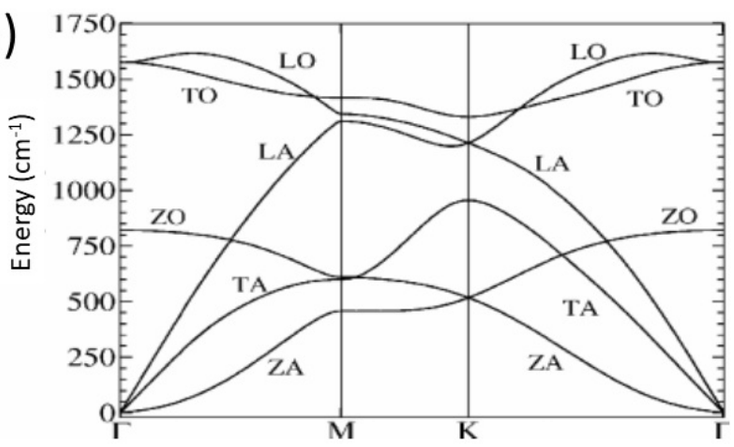
Maximum marks: 10

Full answers. Maximum points indicated.

You may use only the digital form also for this task.

Feel free to scan handwritten notes.

a)



b)

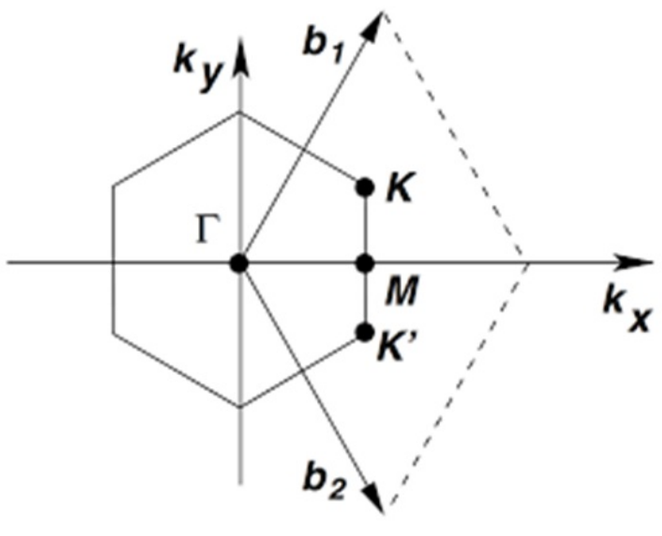


Figure. a) The phonon dispersion relation for graphite.

b) As usual, Γ, M, K denote high symmetry points in the 1st Brillouin zone.

The hexagonal unit cell has a = 2.456 Å and c = 6.694 Å (with $c/2$ = 3.347 Å between adjacent layers).

Note: The energy in the figure is given in "spectroscopy units" of cm^{-1}.

1 cm^{-1} corresponds to 0.000123986 eV.

18

3a) Graphite phonon dispersion I (5 points)

- How many atoms are there per primitive cell? Explain briefly, based on the dispersion relation.

Fill in your answer here

Format

Words: 0

Maximum marks: 5

19

3b) Graphite phonon dispersion II (5 points)

- ZA and ZO in Fig. a) denote out-of-plane acoustic and optical branches, respectively. Based on your knowledge of graphite as a layered material, comment on the frequency ω of the ZO branch compared the other optical modes!

Fill in your answer here

Format | B I U x_2 x^2 I_x | ABC

Words: 0

Maximum marks: 5

20

3c) Graphite phonon dispersion III (10 points)

- Estimate the sound velocity for the LA modes.

Fill in your answer here

Format

Words: 0

Maximum marks: 5

Full answers

You may use only the digital form also for this task.

Maximum points indicated.

Feel free to scan handwritten notes.

The oxides of copper have played a prominent role in the development of solid state physics. Here we will study some features of Cu_2O.

Cu_2O is cubic with the following atomic coordinates for the basis:

Cu: (¼, ¼, ¼), (¼, ¾, ¾), (¾, ¼, ¾), (¾, ¾, ¼)

O: (0,0,0), (½ ½ ½)

21

4a) Cu2O, lattice (5 points)

- Explain shortly the terms *Bravais lattice* and *basis*.
- With the atomic coordinates as given, is the lattice *b.c.c.*, *f.c.c.* or *primitive*?

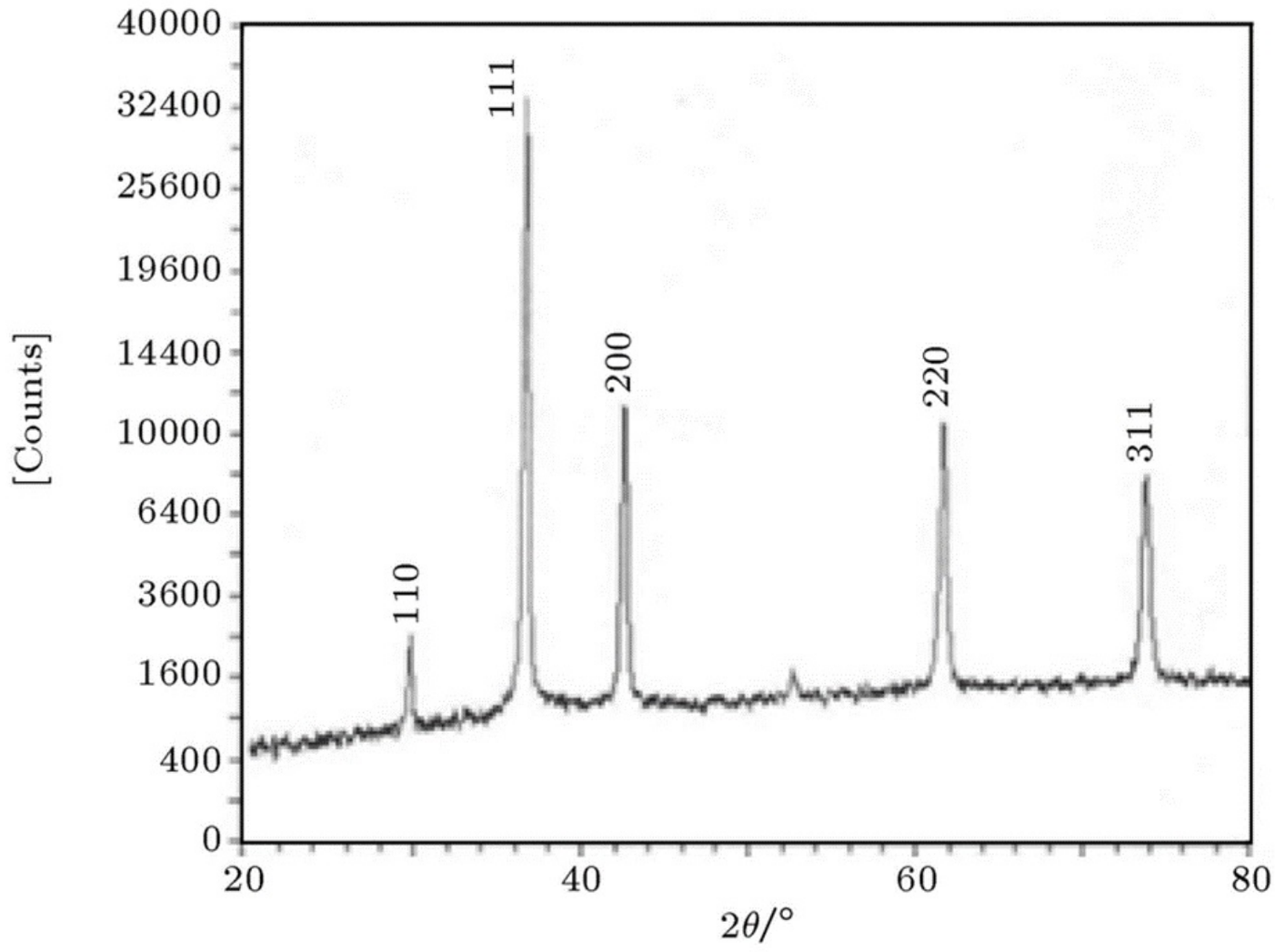
Fill in your answer here

Format | B I U x_2 x^2 I_x | Ω | ∑ | ABC

Words: 0

Maximum marks: 10

22 4b) Cu2O diffraction (10 points)



The powder X-ray diffraction pattern for Cu_2O is given above. The scattering angle is denoted by 2θ. The *111* diffraction peak is at $2\theta = 36.29°$. The side length of the unit cell is $a = 4.288$ Å.

- Based on the information given about the *111* reflection, derive the wavelength of the (approximately monochromatic) X-ray radiation used for the diffraction experiment.
- What information is contained in the peak widths?

Fill in your answer here

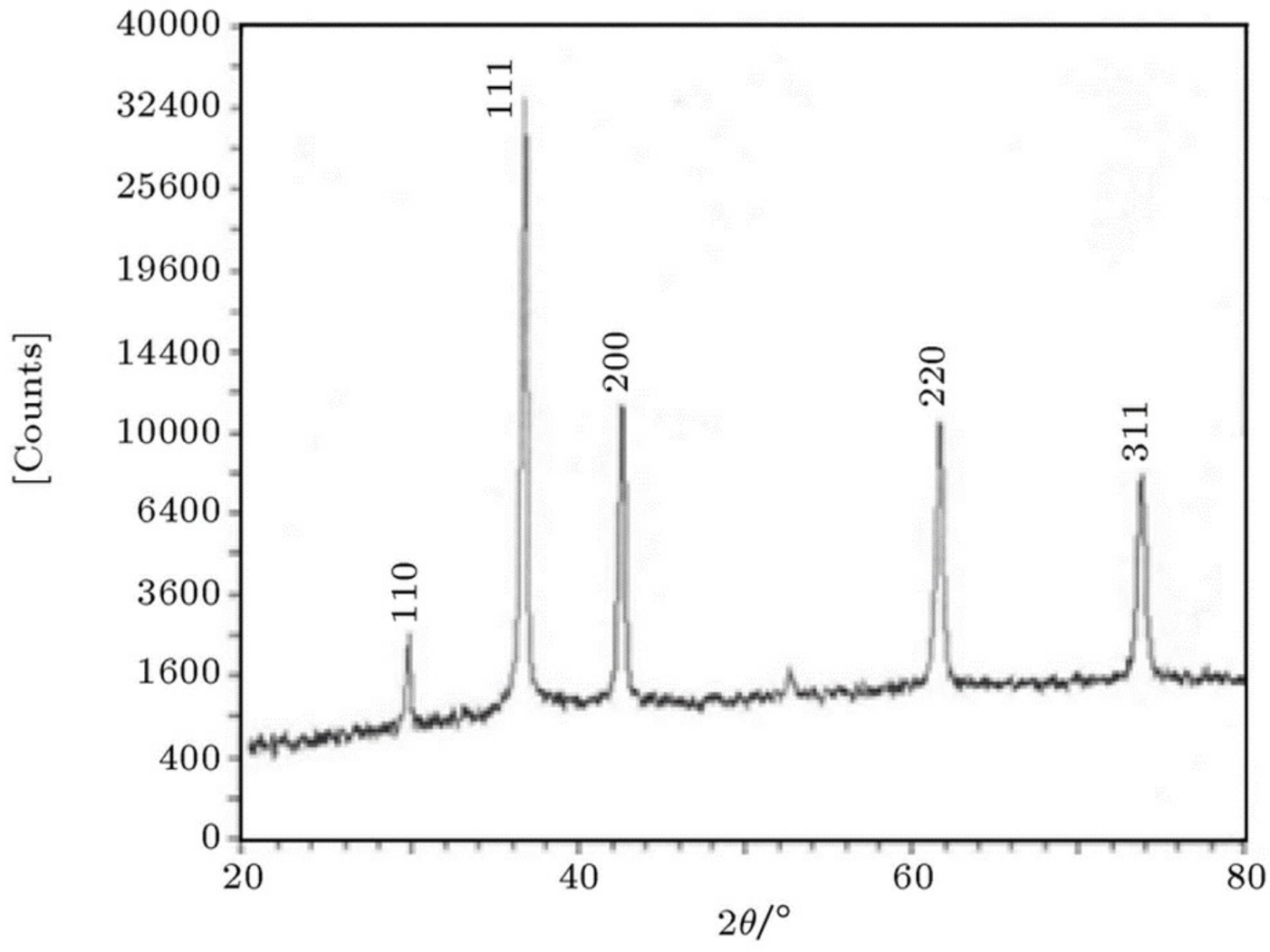
Format

Words: 0

Maximum marks: 10

23

4c) Cu2O structure factor (10 points)



- Derive the general expression for the unit cell structure factor, i.e., starting out with $F(\mathbf{Q}) = \int \rho(\mathbf{r}) \exp(i\mathbf{Q}\cdot\mathbf{r}) d\mathbf{r}$, show that $F_{hkl} = \sum_j f_j \exp(2\pi i(hx_j + ky_j + lz_j))$, where the symbols have their usual meaning.
- Explain in particular how one arrives at the scattering condition $\mathbf{Q} = \mathbf{G}$.
- Explain (calculations not needed) why the $\bar{2}00$ and *210* diffraction peaks are not indicated in the diffractogram.

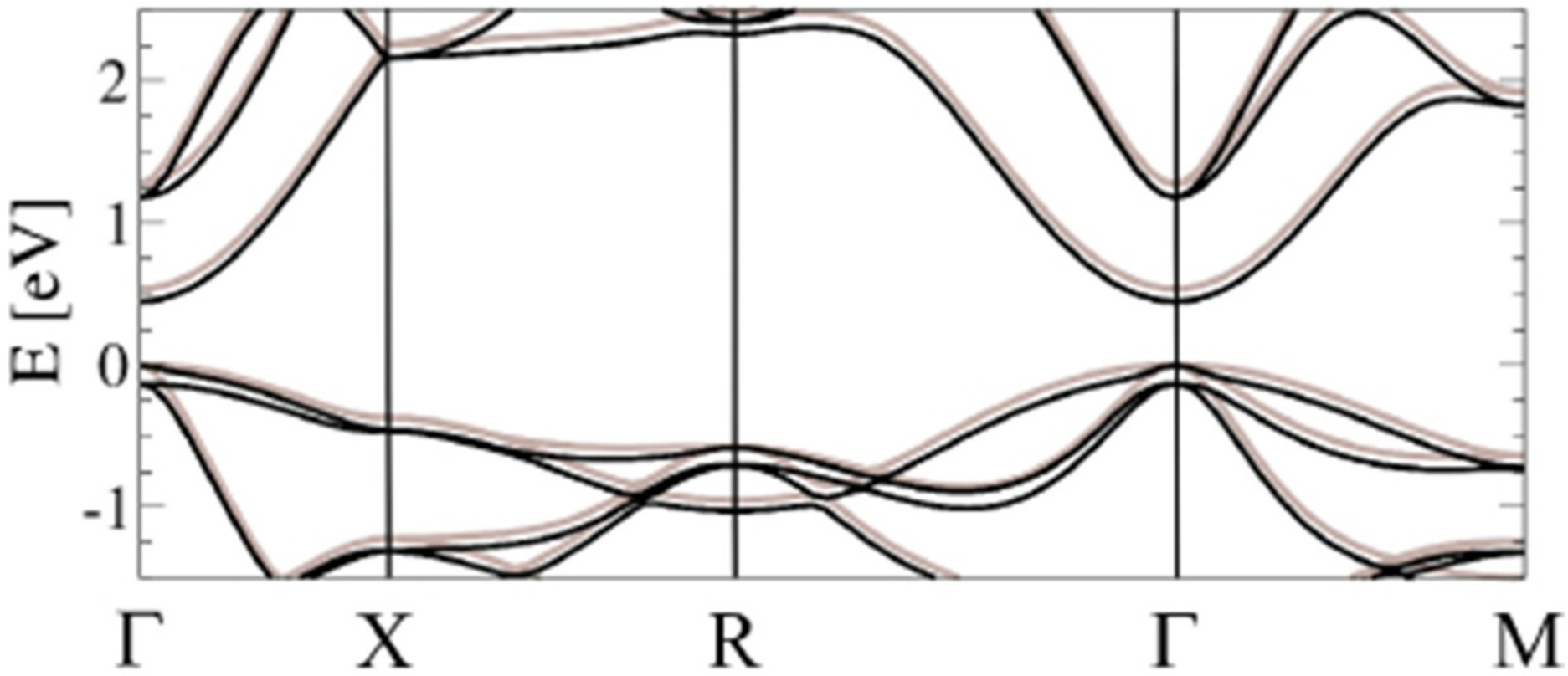
Fill in your answer here

Format

Words: 0

Maximum marks: 10

24 4d) Cu2O band structure (5 points)



The relevant part of the (calculated) electronic band structure of Cu_2O near the Fermi level (at $E = 0$, just above the valence band) is given in the figure. As usual, Γ denotes the center of the 1st Brillouin zone. (The double lines are caused by different assumptions for the bandstructure calculations and should be ignored).

- Based on the band structure, explain whether there is a bandgap, direct or indirect, and whether Cu_2O is a metal, semimetal, insulator or semiconductor.

Fill in your answer here

Format

Words: 0

Maximum marks: 10

25

4e) Indirect bandgap (5 points)

- Explain briefly the consequences of an *indirect* bandgap for the absorption of light, and its relevance to solar cells.
- Explain how the bandstructure of a semimetal differs from a semiconductor and how this difference is revealed in the electronic density of states.

Fill in your answer here

Format | B I U x_2 x^2 I_x | ABC

Words: 0

Maximum marks: 10