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Department of Physics

Examination paper for TFY4220 Solid State Physics

Examination date: 3 June 2020

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

Permitted examination support material: All support material is allowed.

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OTHER INFORMATION

Saving: Answers written in Inspera are automatically saved every 15 seconds.

Cheating/Collaboration: The exam is an individual, independent work.

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Weighting: The multiple choice questions will be equally weighted, with 1 point for a correct answer and 0 points for a wrong answer. No points will be given for uploaded explanations etc.

Submission: Your answer will be submitted automatically when the examination time expires and the test closes, if you have answered at least one question. This will happen even if you do not click "Submit and return to dashboard" on the last page of the question set. You can reopen and edit your answer as long as the test is open. If no questions are answered by the time the examination time expires, your answer will not be submitted.

Withdrawing from the exam: If you wish to submit a blank test/withdraw from the exam, go to the menu in the top right-hand corner and click "Submit blank". This can not be

undone, even if the test is still open.

Accessing your answer post-submission: You will find your answer in Archive when the examination time has expired.

1 # 1.1

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

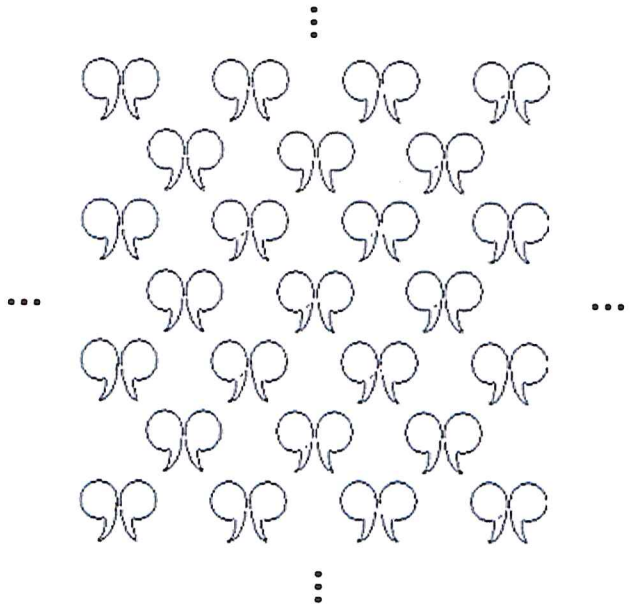
Select one alternative:

- 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 primitive (irreducible; single lattice point) 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 a Cl atom in the center is simple 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.
- The only possibilities for cubic Bravais lattices are simple cubic, face centered cubic and body centered cubic.

Maximum marks: 1

2 1.2

Which of the statements is *correct* regarding this pattern?



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

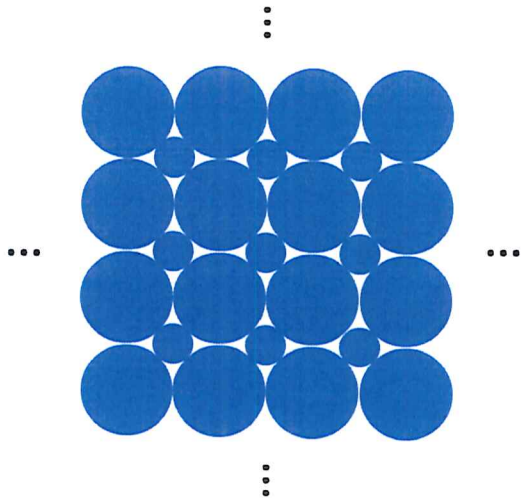
Motif 1: Motif 2:

Select one alternative:

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

Maximum marks: 1

3 1.3



The shown dense 2D packing consists of circular disks of two different diameters in close contact, with their radius ratio allowing the small disks to fit exactly into the void between the larger disks. What is the filling ratio (packing fraction) of the 2D structure shown?

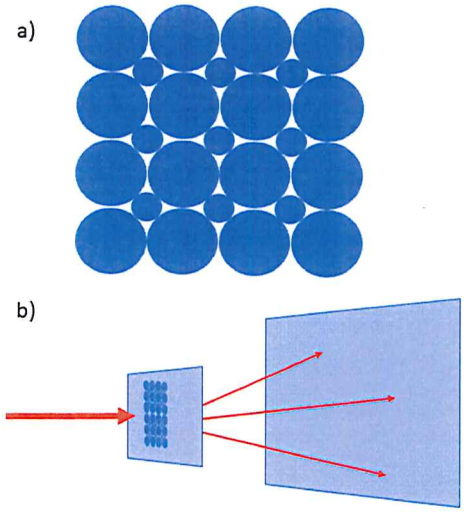
Select one alternative:

- 0.92
- 0.68
- 0.52 (simple cubic)
- 0.74 (same as hexagonal close packed in 3D)
- 0.93

Maximum marks: 1

4 1.4

The shown dense 2D packing consists of circular disks of two different diameters in close contact, with their radius ratio allowing the small disks to fit exactly into the void between the larger disks, see Fig. a). This pattern is used as a μm-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?

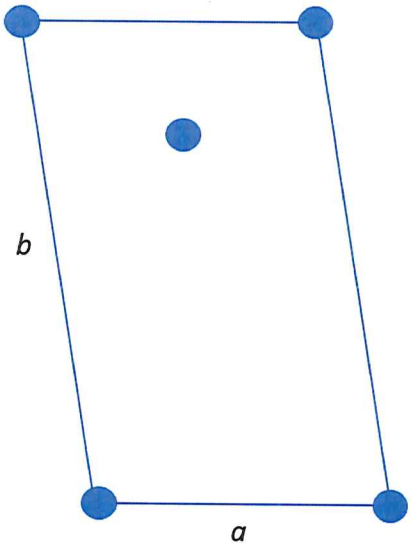
Select one alternative:

- The diffraction pattern will exhibit 6-fold symmetry.
- ✓ The diffraction pattern will exhibit 4-fold symmetry.
- The **Q** = **G** diffraction condition does not apply to this setup.
- The diffraction pattern will not contain information about the relative diameters of the disks.
- The answer depends on how far the detecting plane is from the object.

Maximum marks: 1

5 **1.5**

A primitive 2D unit cell is decorated as illustrated in the figure:



What are the approximate relative coordinates (x_i, y_i) of the atoms in the *basis*?

Select one alternative:

- (0,0); (1,0); (0,1); (1,1); (0.5, 0.5)
- (0,0); (1,0); (0,1); (1,1); (0.5, 0.75)
- (0,0); (0.25, 0.75)
- ✓ (0,0); (0.5, 0.75)
- (0,0); (1,0); (0,1); (1,1); (0.25, 0.75)

Maximum marks: 1

6 1.6

In a powder diffraction experiment, X-rays of energy E = 8040 eV are used. A Bragg diffraction peak is observed at a scattering angle $2\theta = 28.7°$.

What is the corresponding layer spacing d?

Select one alternative:

- ✓ d = 3.11 Å
- d = 1.61 Å
- d = 3.21 Å
- Cannot be answered because the sample orientation is not specified.
- d = 3.11 $Å^{-1}$

Maximum marks: 1

7 **1.7**

The primitive translation vectors of the monoclinic lattice may be taken as $\mathbf{a_1} = a\hat{\mathbf{x}}$, $\mathbf{a_2} = b\hat{\mathbf{y}}$, $\mathbf{a_3} = c\cos(\beta)\hat{\mathbf{x}} + c\sin(\beta)\hat{\mathbf{z}}$.

Find an expression for the reciprocal lattice vector $\mathbf{G}_{20\bar{1}}$.

Select one alternative:

- ✓ $\mathbf{G}_{20\bar{1}} = \frac{4\pi}{a}\left\langle 1, 0, -\frac{\cos\beta}{\sin\beta}\right\rangle - \frac{2\pi}{c\sin\beta}\langle 0, 0, 1\rangle$
- $\mathbf{G}_{20\bar{1}} = \frac{2\pi}{a}\langle 2, 0, -\tan\beta\rangle - \frac{2\pi}{c\sin\beta}\langle 0, 0, 1\rangle$
- $\mathbf{G}_{20\bar{1}} = \frac{4\pi}{a}\left\langle 1, 0, -\frac{\cos\beta}{\sin\beta} - \frac{2a}{c}\right\rangle$
- $\mathbf{G}_{20\bar{1}} = \frac{2\pi}{a}\left\langle 2, 0, -\frac{\cos\beta}{\sin\beta}\right\rangle - \frac{2\pi}{c\sin\beta}\langle 0, 0, 1\rangle$
- $\mathbf{G}_{20\bar{1}} = \frac{4\pi}{a}\left\langle 2, 0, -\frac{\cos\beta}{\sin\beta}\right\rangle + \frac{2\pi}{c\sin\beta}\langle 0, 0, 1\rangle$

Maximum marks: 1

8 Phonons 2.1

For describing a 1D chain of atoms, the following equation can be written down:

$$M\frac{d^2u}{dt^2} = -C_1(u_s - u_{s+1}) - C_1(u_s - u_{s-1}) - C_2(u_s - u_{s+2}) - C_2(u_s - u_{s-2})$$

Here, M is the mass of the atoms, C_1 and C_2 are force constants, and the us denote displacements.

What is described by this equation?

Select one alternative:

- This equation describes optical phonons.
- This is a force balance, including nearest neighbors *only*.
- This is a dispersion relation.
- ✓ This is a force balance, including 2nd nearest neighbors.
- This is a force balance, including 3rd nearest neighbors.

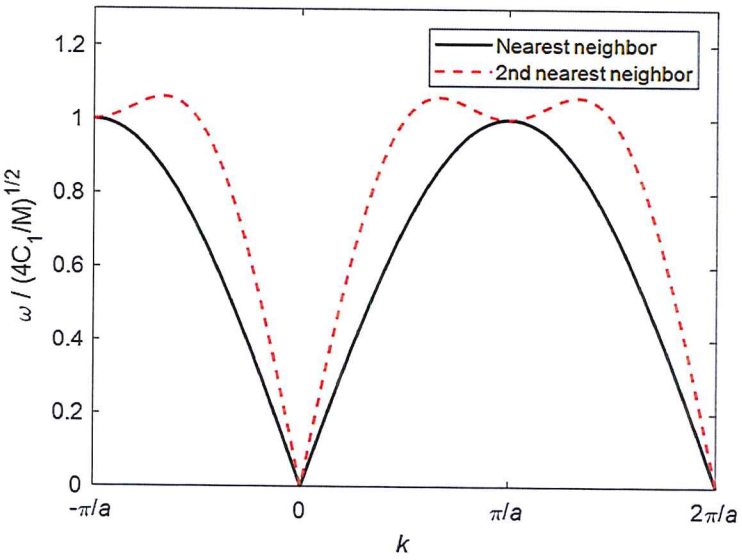
Maximum marks: 1

9 Phonons 2.2

It can be shown that the dispersion relation for phonons on a 1D string with 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.



Which of the following statements is *incorrect* for this 2nd nearest neighbor dispersion relation, as compared to the standard nearest neighbor model?

Select one alternative:

- A qualitatively new feature is that there is now a region with positive k in the 1st Brillouin zone having $v_g < 0$.
- The sound velocity has increased when including the 2nd nearest neighbors.
- ✓ The lattice vibrations are standing waves only at the Brillouin zone boundary.
- The maximum frequency has increased when including the 2nd nearest neighbors.
- The standard dispersion relation for a monatomic 1D-chain is retrieved in the limit $C_2 \to 0$.

Maximum marks: 1

10 Phonons 2.3

In a rectangular 2D lattice with a = 6.90 Å and b = 4.50 Å, three phonons each having wavevector $\mathbf{k}$ = <0.70, 0.90> Å^{-1} merge to become one phonon.

What is the 1st Brillouin zone representation of the $\mathbf{k}$-vector of the resulting phonon?

Select one alternative:

- $\mathbf{k} = \mathbf{0}$
- ✓ $\mathbf{k} = \langle 0.28, -0.09 \rangle \text{ Å}^{-1}$
- $\mathbf{k} = \langle 0.46, 0.70 \rangle \text{ Å}^{-1}$
- $k = |\mathbf{k}| = 3.42 \text{ Å}^{-1}$
- $\mathbf{k} = \langle 2.10, 2.70 \rangle \text{ Å}^{-1}$

Maximum marks: 1

11 Phonon 2.4

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

Select one alternative:

- Silicon has fcc (diamond) structure. It has acoustic and optical phonons because there are two atoms in the primitive unit cell.
- ✓ For a 1D nano structure, the number of possible values of k equals $2N$, where N is the number of unit cells.
- The Einstein model predicts that the heat capacity goes to zero when T goes to zero.
- The equipartition theorem predicts that the phonon heat capacity is constant for all T.
- Aluminium has fcc structure. It has only acoustic phonons because there is only one atom in the primitive unit cell.

Maximum marks: 1

12 Electronics 3.1

When deriving the central equation in 1D, a Fourier expansion of the potential energy is given by $U(x) = \sum_G U_G e^{iGx}$, while the wave function is expanded as $\psi(x) = \sum_k C_k e^{ikx}$.

Which of the following statements is correct?

Select one alternative:

- *G* denotes all reciprocal lattice vectors and is a subset of *k*. *k* is continuous.
- *G* denotes all reciprocal lattice vectors and is a subset of *k*. *k* is quantized.
- By the definition of the reciprocal lattice, exp(i*Gx*) = 1, which simplifies the expression for *U*(*x*).
- *G* and *k* are just book-keeping parameters, both denote the same sets.
- *G* denotes one reciprocal lattice vector, so the summation can be removed.

Maximum marks: 1

13 Electronics 3.2

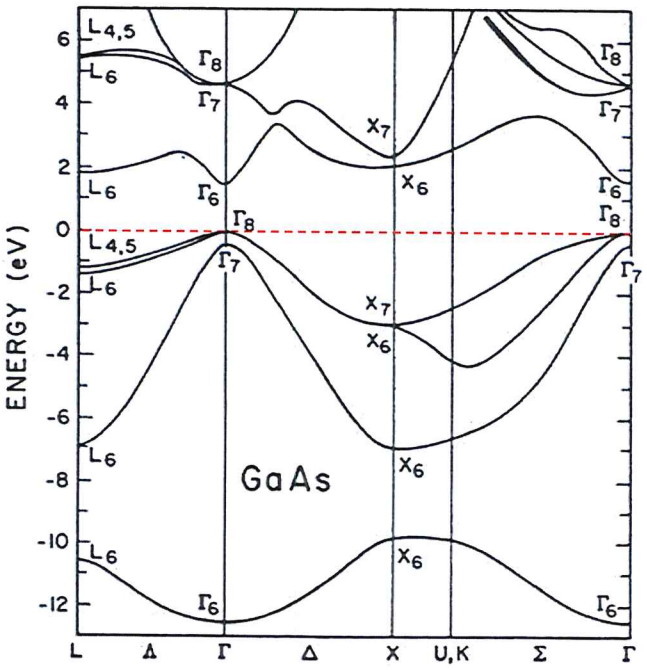
Consider a square 2D piece of metal of length *L*, which we describe with the free electron Fermi model. The square unit cell has sides of length *a* = 5.0 Å. What is the energy *E* of an electron in the corner of the 1st Brillouin zone?
(Choose *E* = 0 at the Γ-point).

Select one alternative:

- $E = m_e c^2$
- $E = \frac{h^2}{m_e a L}$
- $E = \frac{h^2}{2 m_e a^2}$
- ✓ $E = \frac{h^2}{4 m_e a^2}$
- $E = \frac{h^2}{m_e L^2}$

Maximum marks: 1

14 Electronics 3.3



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

Which one of the following statements is *incorrect*?

Select one alternative:

- The bandgap is direct.
- There are hole bands with different hole masses.
- The bandgap is ≈ 1.4 eV.
- ✓ In a direct bandgap semiconductor, phonon-assisted electron transitions cannot exist.
- The bandgap is the result of a periodic potential.

Maximum marks: 1

15 Electronics 3.4

Which of the following statements is *incorrect* regarding the free electron Fermi gas model for an isotropic material?

Select one alternative:

- The model predicts that in *k*-space, the electrons arrange in a Fermi sphere of radius k_F at $T = 0$.
- ✓ A weak periodic potential with the periodicity of the crystal lattice is assumed.
- The model can account for the electronic contributions to the heat capacity.
- The model is quite good for describing the alkali metals.
- The Pauli exclusion principle is contained in the model.

Maximum marks: 1

16 Electronics 3.5

Which of the following statements is *incorrect* regarding the free electron Fermi gas model?

Select one alternative:

- The allowed values of *k* are discrete and equally spaced in *k*.
- The momentum is sharply defined.
- The density of states in *k*-space is given by $\rho_k = (\frac{L}{2\pi})^3$, where *L* is the characteristic length of the 3D specimen.
- The solutions to the Schrödinger equation are given as plane waves.
- ✓ The energy levels are discrete and the spacing between the energy levels increases with energy.

This task was given reduced weight during grading because some of the alternatives are ambiguous.

Maximum marks: 1

17 Electronics 3.6

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

Select one alternative:

- Only electrons near the Fermi level can be thermally excited to higher energy levels at room temperature.
- The entire Fermi sphere shifts in k if an electric field is applied across the specimen.
- The Fermi velocity v_F is of the order of 10^6 m/s.
- ✓ The electrons residing near the surface of the Fermi sphere are not moving in real space at $T = 0$ K.
- Even if the size of the crystal is doubled along one or more dimensions, the Fermi sphere stays the same.

Maximum marks: 1

18 Electronics 3.7

Which of the following statements is *incorrect* for semiconductors?

Select one alternative:

- The dominant (majority) charge carrier can be determined by Hall measurements.
- A semiconductor has an energy gap in its band structure, and the number of electrons exactly fill all states up to the gap at $T = 0$ K.
- ✓ Intrinsic semiconductors always have an equal mobility of electrons and holes.
- Both electrons and holes contribute to charge transport at $T > 0$ K.
- For photovoltaic applications, a direct bandgap gives better quantum efficiency.

Maximum marks: 1

19 Electronics 3.8

Which of the following statements is *incorrect* for semiconductors?

Select one alternative:

- The effective mass of holes can be negative.
- The effective mass of electrons can be negative.
- To describe the conduction band, a starting point is to use the energy dispersion of free electrons, modified with an effective mass.
- The chemical potential of an intrinsic semiconductor is in the middle of the bandgap, provided that the effective masses $m_h^* = m_e^*$.
- ✓ The density of states in the bandgap of an intrinsic semiconductor cannot be zero.

Maximum marks: 1

20 Electronics 3.9

Which of the following statements is *incorrect* for Bloch functions?

Select one alternative:

- ✓ Bloch waves have momentum $\mathbf{p} = \hbar\mathbf{k}$.
- A Bloch function is the general solution of the Schrödinger equation for a periodic potential.
- A superposition of Bloch functions (wave packets) can be assembled to describe localized electrons.
- A Bloch wave consists of a plane wave which does *not* necessarily have the periodicity of the lattice, multiplied by a periodic function which is invariant under lattice translations.
- Measurable quantities (like the probability density) associated with Bloch functions must have the periodicity of the crystal lattice.

Maximum marks: 1

21 **Electronics 3.10**

Consider a weak simple harmonic 1D potential with $U_g = U_{-g} = U$, all other $U_G = 0$. Consider the following version of the central equation, written out for $\boldsymbol{k} \rightarrow \boldsymbol{k} + 5\boldsymbol{g}$, with g being the shortest possible reciprocal lattice vector:

$$\frac{\hbar^2(k+5g)^2}{2m} c_{k+5g} + U c_{k+6g} + Y = 0.$$

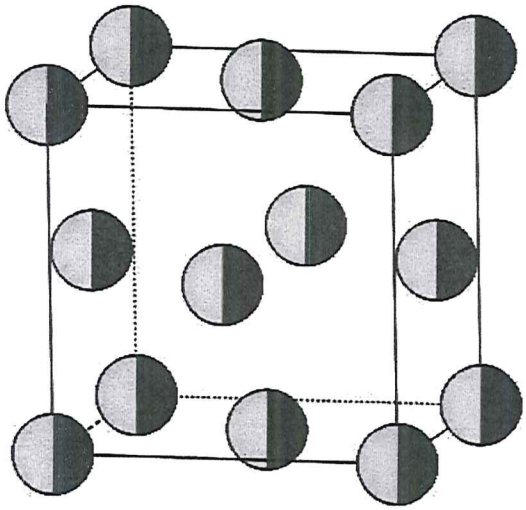
What is the correct expression for Y?
Select one alternative:

- $Y = U c_{k+g}$
- $Y = 0$
- ✓ $Y = U c_{k+4g}$
- $Y = U c_{k+2g}$
- $Y = U c_{k+7g}$

Maximum marks: 1

22 **Au-Cu 4.1**

The high temperature solid phase of 50 atomic % - 50 atomic % Au-Cu alloys has a cubic unit cell, with equal probability of each atomic position of the unit cell to be occupied by a Cu or Au atom, as illustrated in the figure.



The unit cell structure factor can thus be expressed as:

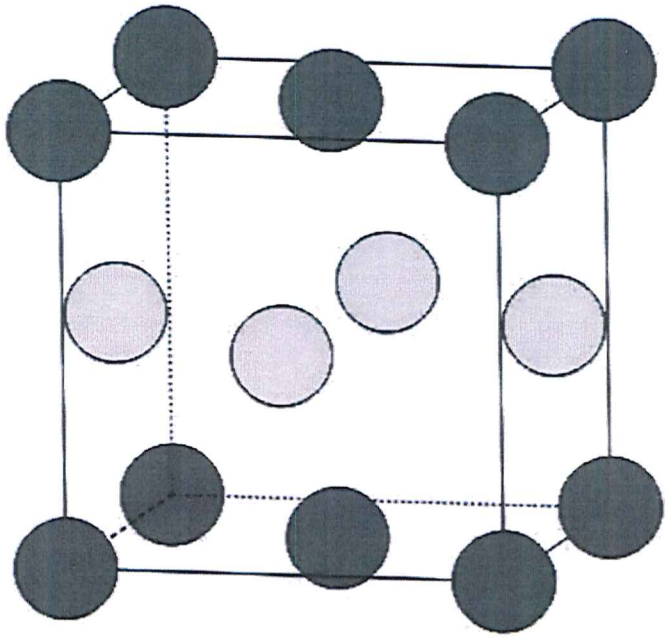
Select one alternative:

- $F_{hkl} = \frac{1}{2}|f_{Cu} - f_{Au}|(1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l})$
- $F_{hkl} = \frac{1}{2}(f_{Cu} + f_{Au})(1 + (-1)^{h+k+l})$
- ✓ $F_{hkl} = \frac{1}{2}(f_{Cu} + f_{Au})(1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l})$
- $F_{hkl} = 0$
- Cannot be defined without knowing the dimensions of the unit cell.

Maximum marks: 1

23 Au - Cu 4.2

The room-temperature solid phase of 50 atomic% - 50 atomic% Au-Cu alloys has a tetragonal unit cell, decorated with Cu or Au atoms, as illustrated in the figure.



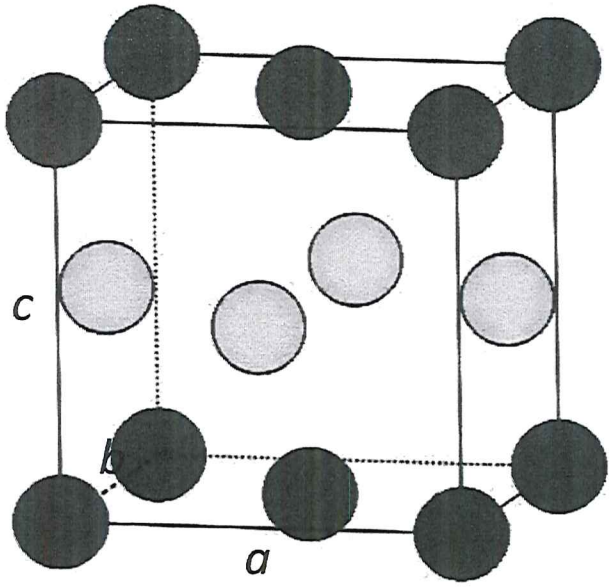
Which of the following statements is *incorrect*?

Select one alternative:

- There is a four-fold rotation axis and several mirror planes present.
- ✓ The symmetry of the unit cell does not change between the high-T (cf. previous problem) and room-T phases.
- Independently of the choice of unit cell, the corresponding basis must contain an equal number of Au and Cu atoms.
- The unit cell depicted in the figure cannot be described as face centered cubic.
- It makes no difference whether the light spheres denote Cu and the dark spheres Au, or vice versa.

Maximum marks: 1

24 **Au-Cu 4.3**



Referring to the figure (same as in task 4.2), find an expression for the unit cell structure factor for the simplified case that $h = k = 0$.
(Assume the "dark" atoms to be Cu).

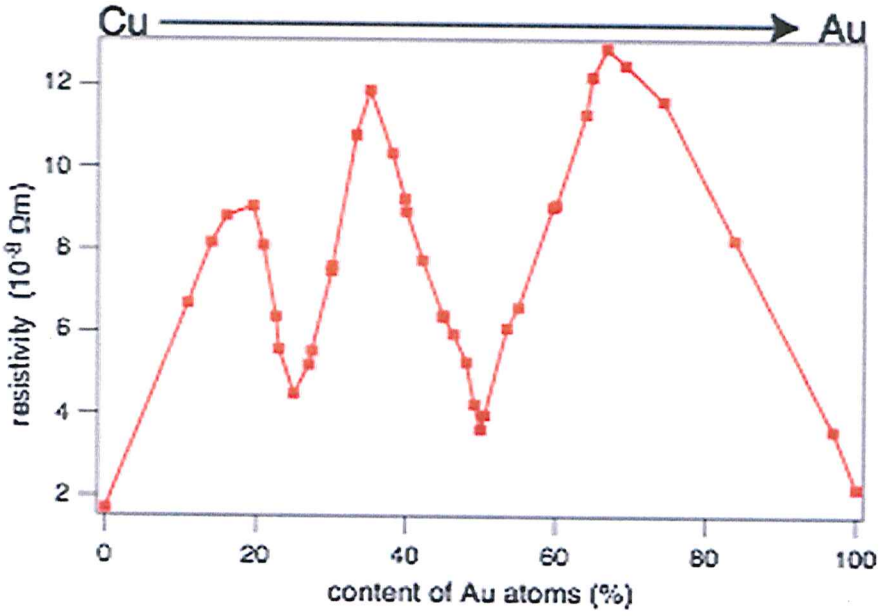
Select one alternative:

- $F_{00l} = 2 + f_{Cu}(-1)^l + f_{Au}(-1)^{l+1}$
- ✓ $F_{00l} = 2(f_{Cu} + f_{Au}(-1)^l)$
- $F_{00l} = 2(f_{Cu} + f_{Au})$
- $F_{00l} = 2f_{Cu} + f_{Au}(-1)^l$
- $F_{00l} = 2(f_{Cu} + f_{Au})^l$

Maximum marks: 1

25 Au-Cu 4.4

The electrical resistivity of Au-Cu alloys at room temperature is plotted in the figure. See also problem Au-Cu 4.2.



Which of the following statements is correct?

Select one alternative:

- The electrical resistivity depends only on the elements present, not the crystal structure.
- The *conductivity* of pure Au is higher than for pure Cu.
- For some Au/Cu mixing ratios, the crystal structure is disordered, giving higher conductivity.
- ✓ At 50-50 atomic % Au-Cu composition, the ordered structure gives a periodic potential and thus less scattering of the electrons.
- Perfect crystals at high *T* allow charge transport by Bloch waves without scattering.

Maximum marks: 1

26 Methods 5.1

Which of the following statements is *incorrect* for transmission electron microscopy?

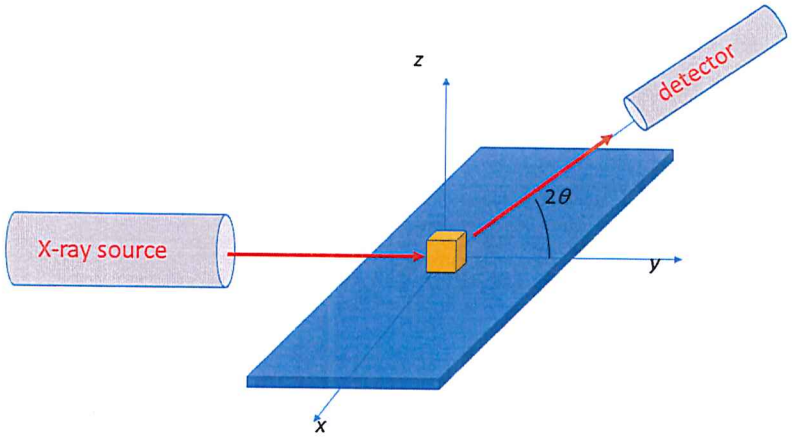
Select one alternative:

- For sufficiently thin and weakly scattering samples, the diffraction pattern can be modeled as the absolute square of the Fourier transform of the crystal field of the object.
- Electron diffraction patterns and real-space microscopy images can be obtained with the same instrument.
- Sub-atomic resolution is possible.
- ✓ The electron wavelength is smaller than 0.01 Å for a common acceleration voltage of U = 200 kV.
- The imaging process is based on the electrons being matter waves.

Maximum marks: 1

27 # Methods 5.2

A single crystal is oriented in the orthogonal laboratory coordinate system , where is the vertical direction. The crystal belongs to the monoclinic crystal system with primitive translation vectors oriented with and , with a = 5.0 Å, b = 7.0 Å, and c = 10 Å. The incoming X-ray beam (=1.542 Å) is directed along . The point detector (sensor) is placed in the $(\mathbf{y}, \mathbf{z})$ plane, and is at an angle $2\theta = 2\arcsin(\frac{\lambda}{2d_{001}})$ with respect to the horizontal, as shown in the figure.



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

Select one alternative:

- ✓ The sample should be rotated an angle $\phi_x = \arcsin(\frac{\lambda}{2d_{001}})$ about the **x**-axis to measure the diffraction peak.
- The question cannot be answered without further information.
- The sample should be rotated an angle $\phi_z = \arcsin(\frac{\lambda}{2d_{001}})$ about the **z**-axis to measure the diffraction peak.
- With the given orientation of the sample, the diffraction condition **Q** = $\mathbf{G}_{001}$ is fulfilled.
- Diffraction from the 001 peak can be seen by choosing the wavelength according to $\lambda = 2d_{001}\sin(2\theta/2)$.

28 Methods 5.3

Which of the following statements is *incorrect* for mathematical properties related to the Fourier transform?

(The figure is for one of the alternatives. The smileys represent repeated objects, the ⊗ symbol denotes convolution, and the blue dots 2D Dirac δ-functions).

Select one alternative:

- The convolution theorem states that the Fourier transform of a product AB equals the Fourier transform of A convoluted by the Fourier transform of B.
- In the Fourier transform, all the information is preserved, including the phase of waves.
- ✓ The convolution theorem can be used to simplify the description of repeated objects, even if differing in orientation, as illustrated schematically in the above figure.
- Convolution can be used for modelling instrument resolution. A «perfect» instrument would have a response function modelled as a Dirac δ-function.
- The Fourier transform of the function

$$f(x) = sin(x), \text{if } x \in (a, b)$$
$$f(x) = 0, \text{otherwise}$$

has infinitely many frequencies.

Maximum marks: 1

29 Methods 5.4

In a neutron diffraction experiment, a neutron wavelength of 1.8 Å is used.

What is the corresponding velocity v of the neutrons?

Select one alternative:

- $v \sim v_{Fermi} \sim 10^6$ m/s
- $v = 0.99c$ (c is the speed of light)
- 2200 m/s
- 2200 km/s
- $v = c$ (c is the speed of light)

Maximum marks: 1

30 # Methods 5.5

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 (as in the TFY4220 X-ray laboratory exercise).

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 corresponds to a strong measured intensity. While the sample is rotated, the intensity measured by the detector is seen to stay constant (within experimental error).

Which alternative can explain these observations?

Select one alternative:

- The sample is a liquid.
- The sample is a single crystal.
- ✓ The sample is an isotropic crystalline powder.
- The sample is a gas.
- The sample is amorphous.

Maximum marks: 1