A1 0.30 Write the formula 1 using the scattering vector q ($q \ll k_i$).

Ответ:

$$I = \frac{I_0}{N^2} \cdot \left(\frac{\sin(Nqa/2)}{\sin(qa/2)}\right)^2 \cdot \left(\frac{\sin(qb/2)}{(qb/2)}\right)^2$$

A2 0.20 Find scattering vector q for the maximum numbered h for a diffraction grating with a period a.

Ответ:

$$q = \frac{2\pi}{a} \cdot h, \quad h \in \mathbb{Z}$$

DISCLAIMER. Here and below we use the notations:
$\mathbb{Z}$ – integer numbers: $\{\dots, -2, -1, 0, 1, 2, \dots\}$
$\mathbb{N}$ – positive numbers: $\{1, 2, \dots\}$

A3 0.20 Let q_1 be the scattering vector for the first maximum. Express q in terms of q_1 for intensity maxima. How are q_1 and a related?

Ответ:

$$q = q_1 \cdot h, \quad h \in \mathbb{Z}$$

$$q_1 \cdot a = 2\pi$$

A4 1.00 Observe the diffraction of samples DG1-DG5. Determine experimentally q_1, and a for each sample. Draw a scheme of your setup, write the quantities you measure, and write down the formulas for the calculations.

$q_1 = \frac{2\pi}{\lambda} \frac{s_N}{NL}$,
where s_N - distance between zero maximum and maximum N; L - distance between DG and screen.

Ответ: DG1: $q_1 = 320 \pm 32\text{mm}^{-1}$ $a = 20 \pm 2\mu\text{m}$
DG2: $q_1 = 130 \pm 13\text{mm}^{-1}$ $a = 50 \pm 5\mu\text{m}$
DG3: $q_1 = 79 \pm 8\text{mm}^{-1}$ $a = 80 \pm 8\mu\text{m}$
DG4: $q_1 = 79 \pm 8\text{mm}^{-1}$ $a = 80 \pm 8\mu\text{m}$
DG5: $q_1 = 79 \pm 8\text{mm}^{-1}$ $a = 80 \pm 8\mu\text{m}$

A5 1.50 Conduct an experiment and determine the a/b ratio for samples DG3, DG4, DG5. Explain your solution using formulas, diagrams, and pictures. It is known that $b \le a/2$.

From formula A1 one could note that intensity I of maximum depends on its number h:

$$I(h) = I_0 \left(\frac{\sin(\pi b/a \cdot h)}{(\pi b/a \cdot h)}\right)^2.$$

Measured intensities for two different maxima gives us a transcendental equation

$$\pi b/a = \arcsin\left(\frac{1}{2}\sqrt{\frac{I(1)}{I(2)}}\sin(2\pi b/a)\right).$$

Root of this equation ($\pi b/a$) could be found numerically.

For DG3 measured intensities are $I(1) = 790mV, \quad I(2) = 630mV$, and solution of equation is $\pi b/a = 0.397$. This leads to $a/b \approx 8.3$, which is quite close to theoretical value 8.

For DG4 and DG5 one could note that each 4th and each 2nd maxima (respectively) are dimmed. That's why $a/b = 4$ for DG4, and $a/b = 2$.

Ответ: DG1: $a/b = 2$
DG2: $a/b = 4$
DG3: $a/b \in [7; 10]$
DG4: $a/b \in [3.2; 4.8]$
DG5: $a/b \in [1.5; 2.5]$

A6 0.70 Write down $\rho(x)$ for the unit cell of the diffraction grating from A1 (Fig. 4A). Use the coordinate system as shown in the figure. Suppose that the unit cell is such that the period of the lattice a is p times the width of the slit b: $a = pb, \quad p \in \mathbb{N}$. Calculate the structure factor $F_A(h)$ for this unit cell for reflex h. Record your answer using h and q_1. What maxima have intensity 0? Write the equation for h for such maxima.

Ответ:

$$\rho(x) = \begin{cases} 1, & x \in [0, b) \\ 0, & x \in [b, a) \end{cases}$$

Ответ:

$$F_A(h) = 2 \cdot \frac{\sin(\pi h/p)}{q_1 h} \cdot e^{i\pi h/p} = \begin{cases} \frac{2\pi}{q_1} \cdot \left(\frac{1}{p}\right), & h = 0 \\ F_1(h), & h \neq 0 \end{cases}$$

Ответ: Equation for zero reflections:

$$h = \pm pm, \quad m \in \mathbb{N}$$

A7 0.70 Consider another unit cell (Fig. 4B) of the diffraction grating. Calculate the structure factor $F_B(h)$ for this unit cell for reflex h. What reflexes of this diffraction grating have an intensity of 0? Write the equation for h for such reflexes.

Ответ:

$$F_B(h) = 2 \cdot \frac{\sin(\pi h)}{q_1 h} \cdot e^{i\pi h} - 2 \cdot \frac{\sin(\pi h/p)}{q_1 h} \cdot e^{i\pi h/p} = \begin{cases} \frac{2\pi}{q_1} \cdot \left(1 - \frac{1}{p}\right), & h = 0 \\ -F_1(h), & h \neq 0 \end{cases}$$

Ответ: Equation for zero reflections:

$$h = \pm pm, \quad m \in \mathbb{N}$$

A8 0.40 These two diffraction gratings described above are illuminated with light of the same intensity. Find the quotients $I_{A,h=0}/I_{B,h=0}$ and $I_{A,h=1}/I_{B,h=1}$.

Ответ:

$$\frac{I_{A,h=0}}{I_{B,h=0}} = \left(\frac{b}{a-b}\right)^2 = \left(\frac{1}{p-1}\right)^2$$

Ответ:

$$\frac{I_{A,h=1}}{I_{B,h=1}} = 1$$

B1 1.00 Find the angle β between the vectors $\vec{q}_1$ and $\vec{q}_2$ and their lengths q_1, q_2. Please note that these vectors must be of minimum length and the angle between them must be $\leq 90^\circ$. Express your answer through the crystal parameters a_1, a_2, α (Fig. 5)

Ответ:

$$|\vec{q}_1| = \frac{2\pi}{a_2 \sin\alpha}, \quad |\vec{q}_2| = \frac{2\pi}{a_1 \sin\alpha}$$

or

$$|\vec{q}_1| = \frac{2\pi}{a_1 \sin\alpha}, \quad |\vec{q}_2| = \frac{2\pi}{a_2 \sin\alpha}$$

Ответ:

$$\beta = \alpha$$

B2 1.00 For crystals A and D, find the complex amplitude modulus $|F(h,k)|$ for the reflex (h,k). Express your answer in terms of a (crystal period) and b (atom size). It is enough to indicate an expression that is true for all reflexes except for the central one ($h = 0, k = 0$)

Ответ:

$$F(h,k) = \int_0^b \int_0^b e^{iq_x x} e^{iq_y y} dx dy = \frac{e^{iq_x b} - 1}{iq_x} \cdot \frac{e^{iq_y b/2} - e^{-iq_y b/2}}{2iq_x a} \cdot 2ae^{iq_y b/2} =$$
$$= \frac{a^2}{\pi^2} \cdot \left| \frac{\sin(\pi hb/a)}{h} \cdot \frac{\sin(\pi kb/a)}{k} \right| \cdot e^{i\pi b(h+k)/a}$$

Ответ: $|F(h,k)| = \frac{a^2}{\pi^2} \cdot \left| \frac{\sin(\pi hb/a)}{h} \cdot \frac{\sin(\pi kb/a)}{k} \right|, \quad h \neq 0, \quad k \neq 0$

B3 0.60 Look at the diffraction patterns of samples UC1-UC4. For each UC1-UC4 sample, experimentally determine the crystal lattice period a_{UC1}, a_{UC2}, a_{UC3}, a_{UC4}.

Ответ: Periods of samples:

$a_{UC1} = 30\mu\text{m}$

$a_{UC2} = 20\mu\text{m}$

$a_{UC3} = 20\mu\text{m}$

$a_{UC4} = 30\mu\text{m}$

B4 0.40 For each UC1-UC4 sample, find the corresponding crystal structure among Fig. 6. Explain your choice using diagrams, pictures and formulas.

Ответ: Corresponding samples:

UC1 - B

UC2 - A
UC3 - D
UC4 - C

B5 0.80 Determine the size of the atom b.

Ответ: $b = 10\mu m$, estimated like in A5 for UC1.

B6 1.20 Observe the diffraction patterns of samples UC5, UC6, UC7. Determine experimentally the parameters a_1, a_2 and the angle α for each sample. Explain which parameters of the diffraction pattern you are using with the help of diagrams and figures.

Ответ: sample UC5:

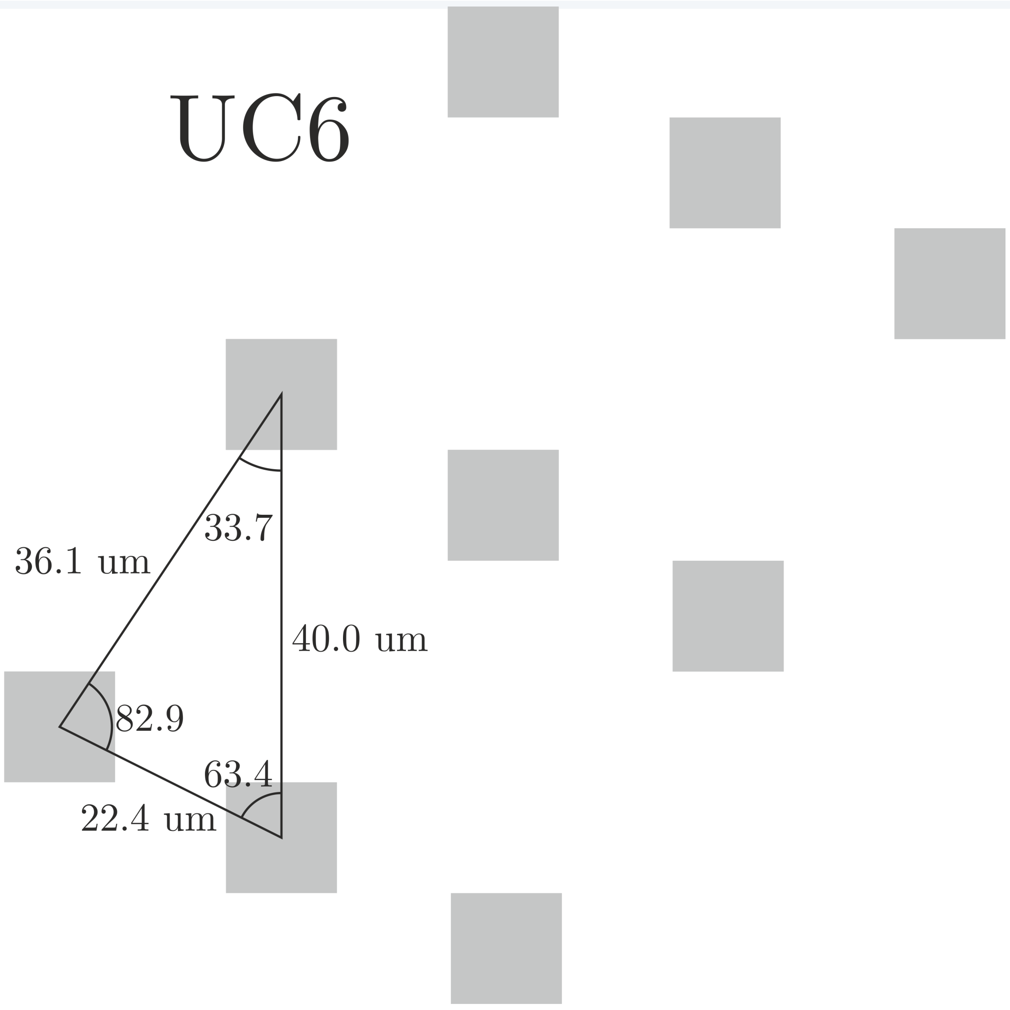
$a_1 = 20\mu\text{m}$, $a_2 = 40\mu\text{m}$, $\alpha = 90^\circ$

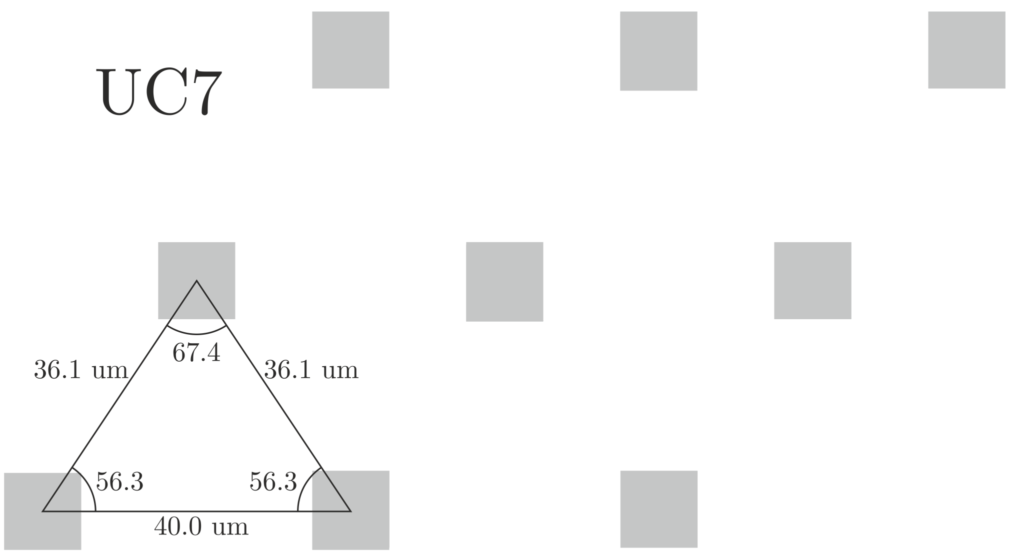
sample UC6:

$a_1 = 36.1\mu\text{m}$, $a_2 = 22.4\mu\text{m}$, $\alpha = 63^\circ$

sample UC7:

$a_1 = 40\mu\text{m}$, $a_2 = 36\mu\text{m}$, $\alpha = 56^\circ$





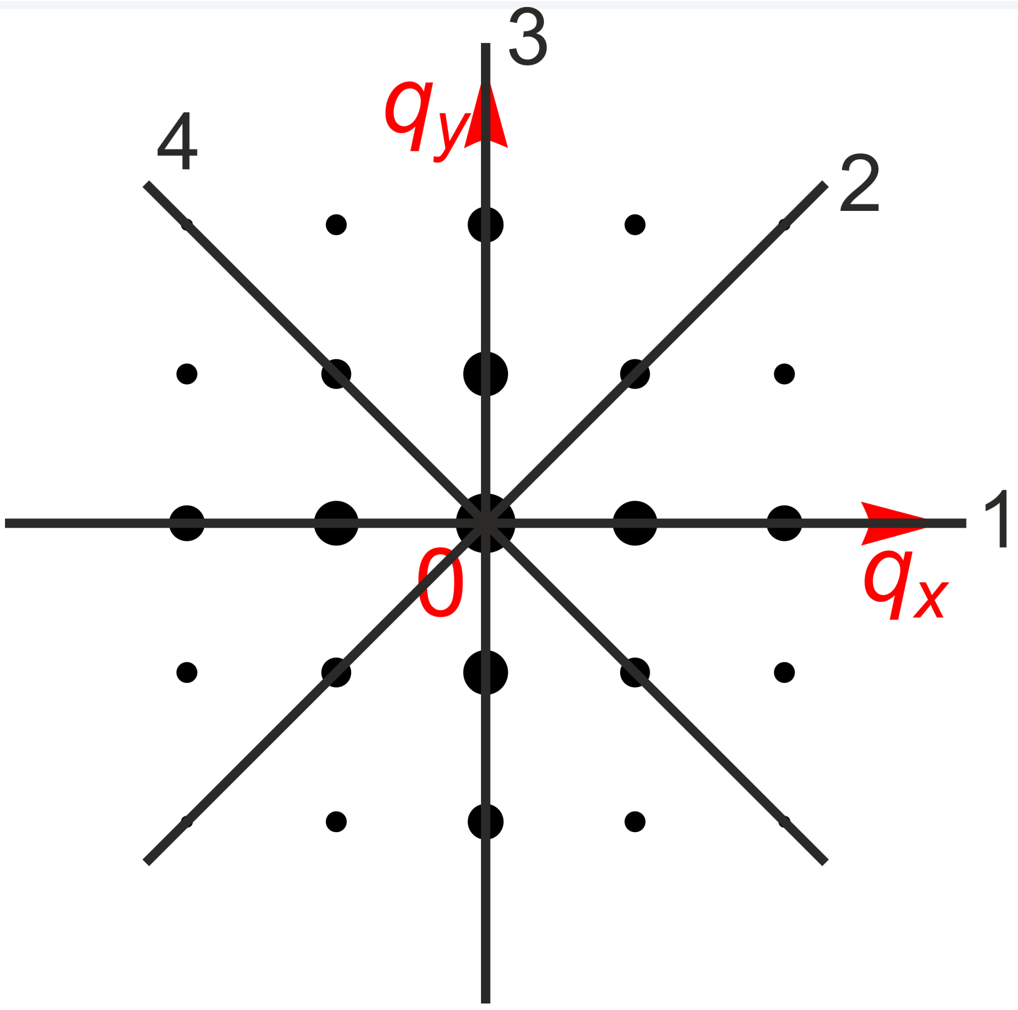
C1 0.30 Specify h and k for the point that will be the center of rotation. What orders of rotational symmetry m are possible for a given image?

Draw all possible axes of mirror symmetry in the image. Name your lines.

Ответ: $h = 0, k = 0$

$m = 1, 2, 4$

All axis of symmetry are presented on figure.



C2 0.20 Specify the equation of the straight line for each axis of mirror symmetry drawn in the previous task. Do not forget to note which equation corresponds to which line.

Ответ: Equations for all possible axis symmetry:

1: $q_y = 0$
2: $q_y = q_x$
3: $q_x = 0$
4: $q_y = -q_x$

C3 0.40 For each rotation symmetry and axis of mirror symmetry, write down the corresponding notation (C_m for rotation and equation for mirror symmetry) and the equation for the intensities $I(q_x, q_y)$, which should take place if this symmetry element is present.

Ответ: Designation (C_m for rotational and equation for axis symmetry) and equation on intensities $I(q_x, q_y)$

C_1: $I(q_x, q_y) = I(q_x, q_y)$

C_2: $I(q_x, q_y) = I(-q_x, -q_y)$

C_4: $I(q_x, q_y) = I(-q_y, q_x)$

$q_y = 0$: $I(q_x, q_y) = I(q_x, -q_y)$

$q_x = 0$: $I(q_x, q_y) = I(-q_x, q_y)$

$q_x = q_y$: $I(q_x, q_y) = I(q_y, q_x)$

$q_x = -q_y$: $I(q_x, q_y) = I(-q_y, -q_x)$

C4 0.20 Write down the equation for the intensities of the reflexes (h,k) and $(-h,-k)$. What symmetry from question C1 corresponds to this equation? Explain your answer.

Structure factor for reflex $-h,-k$:

$$F(-h,-k)=\int\rho(x,y)e^{-i(q_1hx+q_2ky)}dxdy=\left(\int\rho(x,y)e^{-i(q_1hx+q_2ky)}dxdy\right)^*=F^*(h,k).$$

Here F^* is a complex conjugate of F. This property of $-h,-k$ reflex is only possible because $\rho(x,y)$ is real function.

Intensities are equal

$$I(-h,-k)=F(-h,-k)F^*(-h,-k)=F^*(h,k)F(h,k)=I(h,k).$$

Ответ: Equation on intensities

$I(-h,-k)=I(h,k)$

Which symmetry corresponds? C_2

C5 0.40 Using the definition of the structure factor and symmetry find the structural factors $f_2(q_x,q_y)$, $f_3(q_x,q_y)$, $f_4(q_x,q_y)$ for crystals 2, 3, 4, respectively. Express your answer in terms of the structure factor $F(q_x,q_y)=f_1(q_x,q_y)$ of crystal 1.

Let $\rho(x,y)$ be unit cell for initial crystal. Structure factor for it is:

$$F(q_x,q_y)=\int_{-x_0}^{x_0}\int_{-y_0}^{y_0}\rho(x,y)e^{i(q_xx+q_yy)}dxdy,$$

here $x_0=y_0=a/2$, a – is a period of lattice. Below limits are presented only when necessary.

For symmetry $x=0$ unit cell is $\rho_2(x,y)=\rho(-x,y)$, structure factor is

$$f_2(q_x,q_y)=\int_{-x_0}^{x_0}\int_{-y_0}^{y_0}\rho_2(x,y)e^{i(q_xx+q_yy)}dxdy=\int_{-x_0}^{x_0}\int_{-y_0}^{y_0}\rho(-x,y)e^{i(q_xx+q_yy)}dxdy=$$
$$=\int_{x_0}^{-x_0}\int_{-y_0}^{y_0}\rho(x,y)e^{i(-q_xx+q_yy)}d(-x)dy=F(-q_x,q_y).$$

For symmetry $x=y$ unit cell is $\rho_3(x,y)=\rho(y,x)$, structure factor is

$$f_3(q_x,q_y)=\int\rho_3(x,y)e^{i(q_xx+q_yy)}dxdy=\int\rho(y,x)e^{i(q_xx+q_yy)}dxdy=$$
$$=\int\rho(x,y)e^{i(q_yx+q_xy)}dydx=F(q_y,q_x).$$

Point (x,y) moves to new position $(x',y')=(x+x_1,y+y_1)$. That's why $\rho_4(x',y')=\rho(x,y)$.

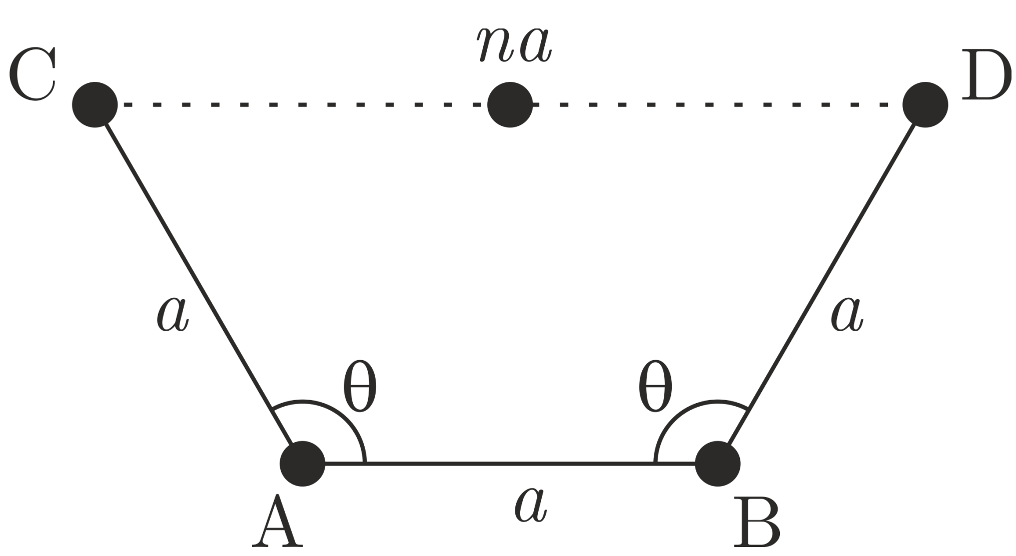
$$f_4(q_x,q_y)=\int\rho_4(x',y')e^{i(q_xx'+q_yy')}dx'dy'=$$
$$=\left(\int\rho(x,y)e^{i(q_xx+q_yy)}dxdy\right)e^{i(q_xx_1+q_yy_1)}=F(q_x,q_y)e^{i(q_xx_1+q_yy_1)}.$$

Ответ: $f_2(q_x,q_y)=F(-q_x,q_y)$

$f_3(q_x,q_y)=F(q_y,q_x)$

$f_4(q_x,q_y)=F(q_x,q_y)\cdot e^{i(q_xx_1+q_yy_1)}$

C6 0.50 Consider an arbitrary 2D crystal (Fig. 5). Indicate what orders of m symmetry of rotation can be in 2D crystals. Explain the answer.



Let's consider two nearest atoms A and B (fig.), that means $\vec{AB}$ – lattice vector, $|\vec{AB}| = a$. If rotational symmetry of order m is present, atom C could be obtained from B by rotation by angle $\theta = \frac{2\pi}{m}$. The same way gives atom D from atom A. These two atoms C and D should also be connected by translation symmetry, it means $\vec{CD} = n \cdot \vec{AB}, \quad n \in \mathbb{Z}$.

It leads us to equation

$$\cos\theta = \frac{1-n}{2}.$$

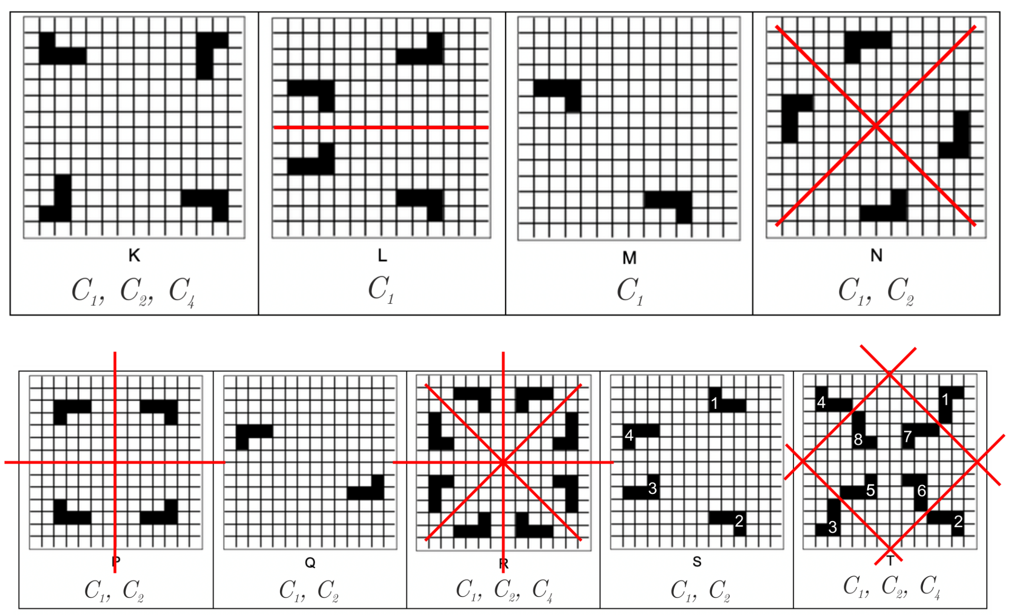
All possible n, $\cos\theta$, θ, m are listed in table.

n	$\cos\theta$	θ	m
-1	1	$0°$	1
0	$1/2$	$60°$	6
1	0	$90°$	4
2	$-1/2$	$120°$	3
3	-1	$180°$	2

Ответ: All possible rotational symmetries: C_1, C_2, C_3, C_4, C_6.

C7 [0.90] Determine what symmetries the crystals with unit cells K, L, M, N, and P, Q, R, S, T have. (Fig. in the answer sheet). Draw the axes of mirror symmetry, at the bottom of the picture indicate which rotational symmetries are present on it.

Symmetries of unit cells:



C8 [0.80] Observe the diffraction patterns of the samples PG 1, 2, 5, 8. These samples correspond to the unit cells K, L, M, N. Determine what symmetries the given diffraction patterns have. Find the correspondence between patterns and unit cells.

PG	$q_x = 0$	$q_y = 0$	$q_x = q_y$	$q_x = -q_y$	C_4
1	+/- *	+			
2					
5			+	+	
8					+

For PG1 vertical axis of symmetry (q_x=0) must be presented theoretically, but real diffraction pictures could be without that symmetry.

Ответ: One needs to match symmetries of unit cells and diffraction patterns.

PG1 - L
PG2 - M
PG5 - N
PG8 - K

C9 1.00 Observe the diffraction of the samples PG 3, 4, 6, 7, 9. These samples correspond to the unit cells P, Q, R, S, T. Find the correspondence between samples and unit cells. Explain your solution using formulas, diagrams and pictures.

PG	$q_x = 0$	$q_y = 0$	$q_x = q_y$	$q_x = -q_y$	C_4
3	+	+			
4	+	+	+	+	+
6	+	+	+	+	+
7					
9	+	+			

Diffraction patterns from PG4 and PG6 have C_4 symmetry (as unit cells R, T), and all other don't have. In this group symmetries are not enough to match unit cells and diffraction patterns. One needs to use sum rule and to understand that absences are presented for unit cells S and T (as for PG6 and PG9).

PG9. Elements are designated as on fig. Elements 2, 3, 4 were obtained by C_2 symmetry and move.

$$f_1(h,k) = F(h,k).$$

$$f_2(h,k) = F(-h,-k)e^{i5\pi h/7}.$$

$$f_3(h,k) = F(-h,k)e^{-i\pi(2h/7+k)}.$$

$$f_4(h,k) = F(h,-k)e^{-i\pi(h+k)}.$$

For reflexes $(0,k)$

$$f_{PG9}(0,k) = (1+\cos(\pi k))\left(F(0,k)+F(0,-k)\right),$$

each odd $k = 2n+1, n \in \mathbb{Z}$ is absent. The same is true for another axis $(h,0)$.

\textbf{PG6.} Let $f_1(h,k) = F(h,k)$. Element 5 could be obtained by mirroring $x = y$ and by moved by $(-a/2, -a/2)$, that's why $f_5(h,k) = F(k,h)e^{-\pi(h+k)}$. Each next pair of elements were obtained by rotating 90°.

Structure factors

$$f_1 + f_5 = F(h,k) + F(k,h)e^{-\pi(h+k)}$$

$$f_2 + f_6 = F(k, -h) + F(h, -k)e^{-\pi(h-k)}$$

$$f_3 + f_7 = F(-h, -k) + F(-k, -h)e^{-\pi(-h-k)}$$

$$f_4 + f_8 = F(-k, h) + F(-h, k)e^{-\pi(-h+k)}$$

For $(0, k)$

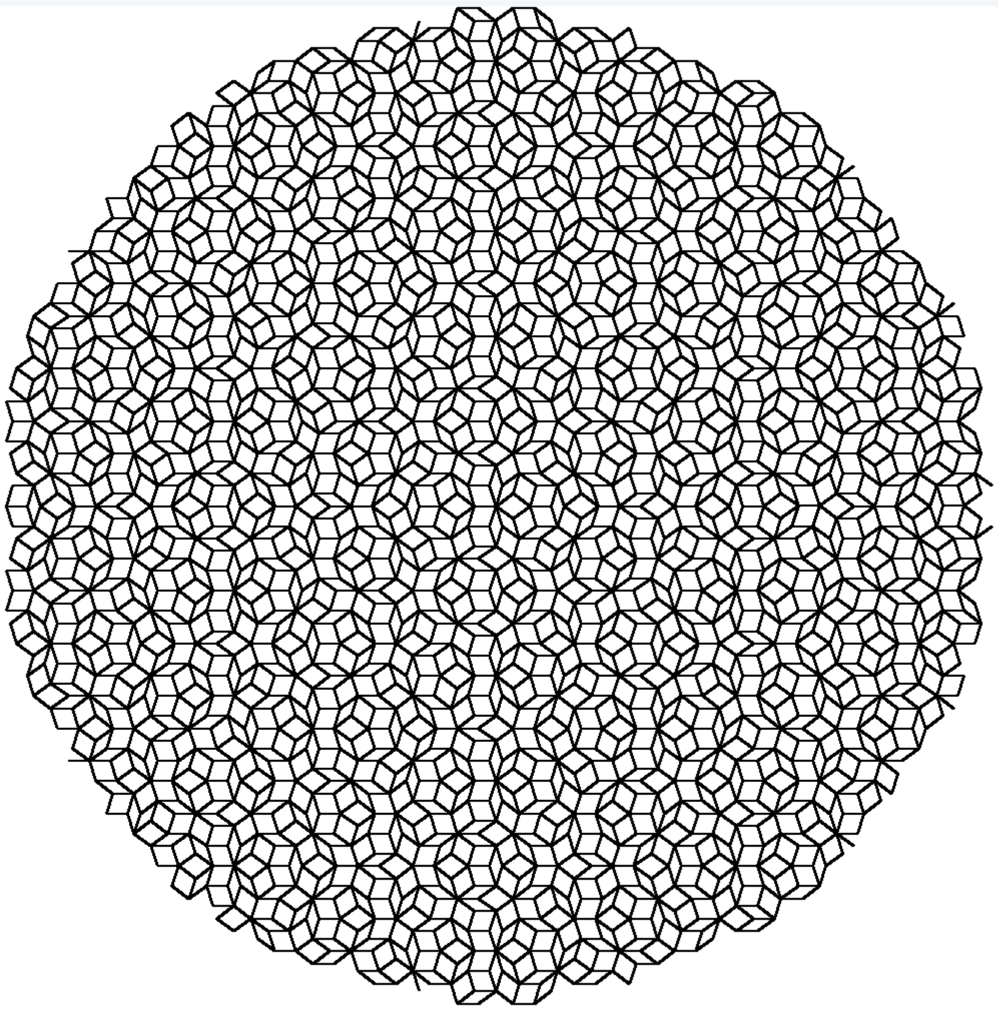
$$f_{PG6}(0, k) = (1 + \cos(\pi k)) \cdot (F(0, k) + F(k, 0) + F(0, -k) + F(-k, 0)),$$

each odd $k = 2n + 1, n \in \mathbb{Z}$ is absent. The same is true for another axis $(h, 0)$.

Ответ: PG3 - P
PG4 - R
PG6 - T
PG7 - Q
PG9 - S

C10 [0.30] Observe the diffraction pattern of the UC8 sample. Could this sample be a crystal? Explain your answer.

Ответ: No. Diffraction picture has symmetry C_5. Transnational symmetry for C_5 is not possible.



Structure used as UC8

D1 [1.00] The crystal (MR0 or MR2) is illuminated with light with an intensity of I_0. Find the intensity of the maximum at $\vec{q} = 0$.

Electric field is $E_0 = \sqrt{I_0}$ in plane exactly before the diffraction grating. Electric field of the reflex $\vec{q} = 0$ is proportional to transparent area of an unit cell and should be E_0 if the whole unit cell is transparent (i.e. there is no any diffraction grating):

$$E = \frac{N_{transparent}}{N_{all}} E_0.$$

Intensity

$$I = \left(\frac{N_{transparent}}{N_{all}}\right)^2 I_0.$$

Ответ:

$$I_{MR0} = \left(\frac{5}{16}\right)^2 \cdot I_0$$

$$I_{MR2} = \left(\frac{7}{16}\right)^2 \cdot I_0$$

D2 2.00 Determine the structure of the unit cell of the MR1 crystal. The MR1 crystal has one of the indicated units cell (Fig. 12). Describe your solution.

MR1

k \ h	−2	−1	0	1	2
2	5.7	19.1	1.6	24.6	15.8
1	36.5	49.2	40.2	3	20.8
0	2.3	20	336	33.5	0.9
−1	22	3.1	23.2	46.5	25.5
−2	2.9	23.9	2	38.5	7.3

One needs to measure intensities $I(h, k)$ of each reflexes $|h| \leq 2$, $|k| \leq 2$ of MR1.

Transparency of a square with position (χ, γ):

$$\rho(\chi, \gamma) = \sum_{h=-2}^{2} \sum_{k=-2}^{2} \sqrt{I(h,k)} \cdot e^{i\varphi(h,k)} \cdot \exp\Big(-2\pi i \left(\frac{\chi}{4} h + \frac{\gamma}{4} k\right)\Big),$$

here $\chi \in 0, 1, 2, 3$, $\gamma \in 0, 1, 2, 3$.

Because $\rho(\chi, \gamma) \in \mathbb{R}$, its enough to calculate only real part:

$$\rho(\chi, \gamma) = \sum_{h=-2}^{2} \sum_{k=-2}^{2} \sqrt{I(h,k)} \cdot \cos\Big(\varphi(h,k) - \frac{\pi}{2}(\chi h + \gamma k)\Big).$$

MR1

γ \ χ	0	1	2	3
3	5.4	4.4	22.6	−9.7
2	−1.7	58.	−13.5	61.1
1	6.	49.1	61.9	−14.4
0	53.8	12.7	−7.5	5.1

Calculated transparencies for MR1 are on figure. It is not necessary to calculate whole 16 squares. One needs to calculate transparency of squares (0,0), (3,3) to understand which values corresponds to transparent and non-transparent values. After that square (3, 2) should be evaluated. It has value close to transparent, that's why structure X is the answer.

Ответ: Unit cell of MR1 - X.

X

D3 2.00 Determine the unit cell structure of the MR2 crystal. The structure of MR2 is similar to MR0: two non-transparent squares have become transparent.

The same formula should be used to find structure of MR2. Intensities of diffraction patterns and calculated transparencies for MR2 are shown on figures

MR2

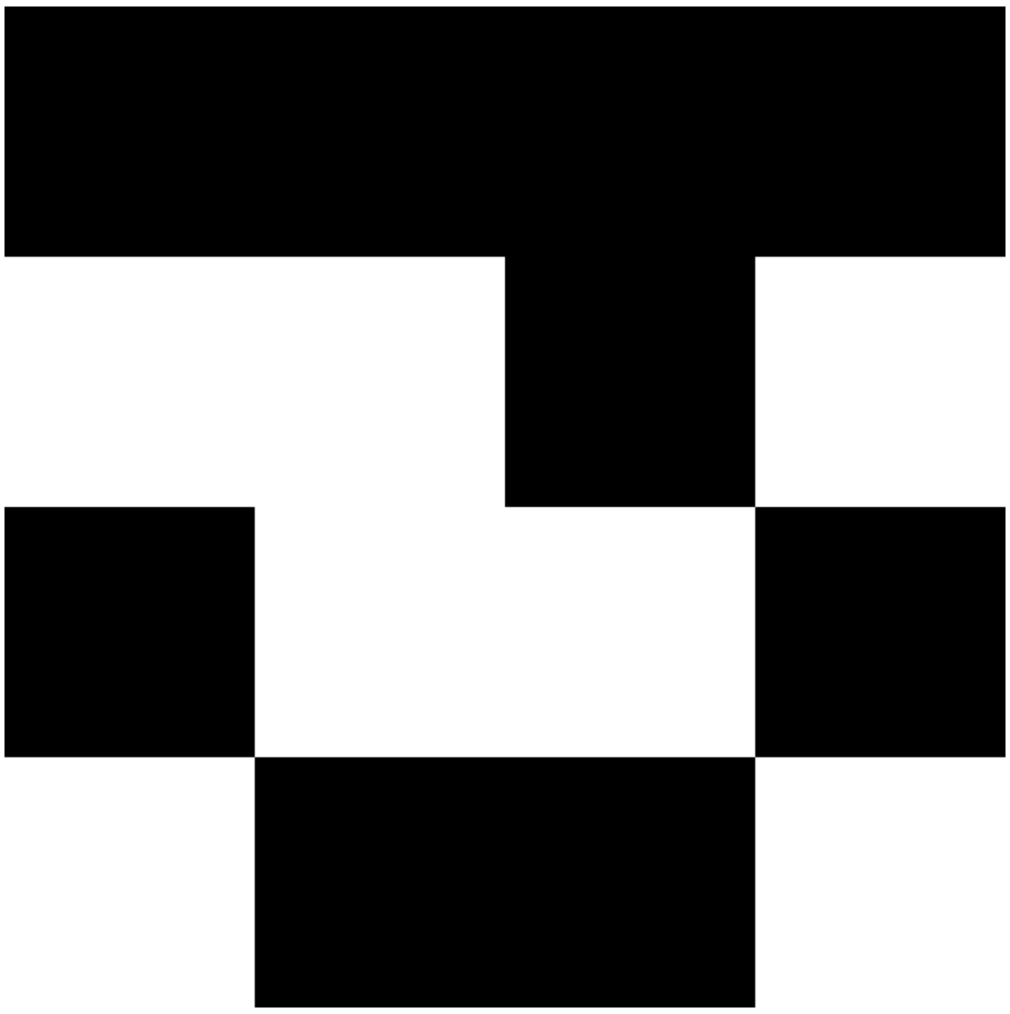
k \ h	−2	−1	0	1	2
2	2	43.3	45.2	39.7	8.9
1	7.2	8.5	69.8	47.9	3.2
0	8.8	11.7	508	4.7	1.7
−1	1.3	40.4	69.7	10	9.3
−2	1.7	56.9	25.8	54.8	1.3

MR2

γ \ χ	0	1	2	3
3	−10.5	5.8	7.3	−19.4
2	41.5	65.3	2.6	57.9
1	−12.6	46.6	69.1	−0.4
0	54.7	11.9	−5.9	46.7

Because it is known that two non-transparent squares become transparent one needs to calculate transparency only for 11 black squares. Two of them (0, 2) and (3,0) are transparent for MR2.

Ответ: Unit cell of MR2 is on figure:



2020 -- We are what they grow beyond.