University of Kasdi Merbah - Ouargla -

Faculty of Mathematics and Material Sciences

Department of Physics

Second Year Physics

2024-2025

Series of exercises and problems - Physics of Crystallography - No. 04

Exercise 1:

-1) What is the difference between reflection and diffraction?

-2) Why there are two types of rays in the X-ray spectrum emitted by any target material?

-3) What is the difference between a single-crystal, polycrystalline, and powder sample.

Exercise 2:

List in the following table the most important features of some experimental methods used in the study of crystal structures:

Method	Sample	(θ)Movement of	Wavelength(λ)	Detector	Results
Laue					
Rotating Crystal					
Debye-Sherrer					

Exercise 3:

The energy of an X-ray photon is given in electron volts, in terms of wavelength, by the following relation: $E = \frac{12400}{\lambda}$

1- State the energy range of X-rays used in crystallography.

2- Find the required voltage to produce X-rays by accelerating electrons, to collide with a copper target with an efficiency of 0.3%.

3- Determine a range of atomic numbers (Z) for elements that can be used as anticathode to produce X-rays at a voltage of (500 kV) for a crystallographic structural investigation.

Exercise 4:

Calculate the structure factor F_{hkl} for all structures in the cubic mono-atomic system.

-1) Deduce the constructive interference and extinction rules for each case.

-2) Write both N and F_{hkl} for the first ten lines of each structure in a table.

-3) Repeat the same question for the diamond structure.

Exercise 5:

Consider the appearance of all possible diffraction peaks for a powder substance of sodium chloride crystals.

1- Find the first six values of the diffraction angle θ .

2- If a=5.64 Å, and λ=1.54 Å. estimate the radiation intensity $I(\theta)$ and give an indexation for these diffraction plans.

Exercise 6:

In an X-ray diffraction study using the Debye-Schährer method on a powder of an unknown structure, a 240 mm film shows diffraction circles whose distance L follows 46.7 / 67.4 / 99 / 120 / 126.8 / 155.8 / 182 / 192.9. If the wavelength used is $\lambda_{K\alpha}$ of copper, identify this structure and its parameters.

Exercise 7:

In a study of diffraction diagrams I(2θ) of two unknown structure compounds, we obtained the following table:

Line number (peaks)		1	2	3	4	5	6	7	8
Structure 1	$2\theta°$	40.48	58.74	73.66	87.82	102.4	115.89	132.6	154.58
	$I\%$	100	14.90	26.00	13.99	18.01	8.55	7.02	8.10
Structure 2	$2\theta°$	33.50	38.88	56.15	67.01	70.40	83.44	92.97	96.18
	$I\%$	2.01	100	53.22	3.02	20.95	11.20	0.54	15.82

1- Determine the Bravais lattice for each structure.

2- Estimate the uncertainty in the lattice parameter .

3- Using the table below, Guess what elements or compounds were studied.

Element/Compound	*Al*	*Ca*	*Mo*	*Pb*	*□-Sn*	*NaF*	*MgO*	*TiO*
Cell parameter	4.049	5.588	3.147	4.950	6.491	4.634	4.213	4.177

Exercise 8:

AB compound crystallizes in the FCC structure, where the cations charge A^{+z} is +Ze and the charge of the anions B^{-z} is –Ze, considering the attractive energy resulting from the electrostatic potential between each ion. Prove that the crystal binding energy can be written as: $E_A(r) = -\frac{1}{4\pi\epsilon_0}\frac{Z^2e^2}{r}M$

Where M is a convergent series called Madelung's constant, and r is the distance of neighboring atoms.

1- Find an approximate value for this constant in the NaCl structure case.

2- We impose the repulsion energy of Born-Landé model as follows: $E_R(r) = Br^{-n}$ give an expression for the constant B, then determine its value if you know that n is related to the Born-Landé factor. The value of which depends on the atomic structure of the noble gases that have a similar structure to the understudy ions, as shown in the table:

Ion configuration	He	Ne	Ar	Kr	Xe
n	5	7	9	10	12

Exercise 9:

For an inert gas crystal in the FCC structure, calculate the distance R_0 of the nearest neighbor and the cell volume V_0 at equilibrium, then find an expression for the volume compressibility of the crystal at constant temperature.