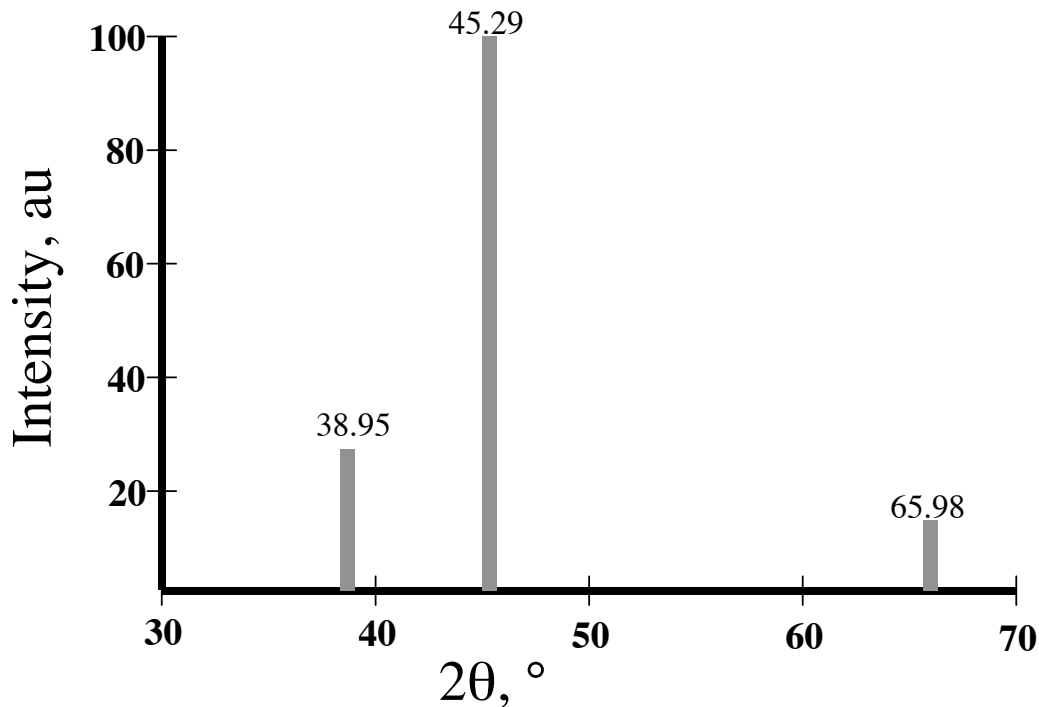


Supplemental Problems for Chapter 5



1) The figure above shows a schematic diffraction pattern for a cubic material, recorded with an X-ray wavelength of 1.54 Å.

- (i) Determine if it is cubic P, I, or F.
- (ii) Estimate the lattice parameter.
- (iii) Is the sample textured? If so, specify the preferred orientation.

2) In the diffraction pattern of a cubic P crystal, which set of planes, (hkl), produces the fifth peak in the pattern (that peak observed at the fifth smallest value of θ). Which set produces the eighth peak?

3) The following questions are about the AuCd structure. For details, see the data in Table 3B.42

- (i) What systematic absences are caused by the a and 2_1 operators in this space group?
- (ii) Describe how you would use a powder diffraction pattern of this material to measure values for a , b , and c .
- (iii) Describe how you would use a powder diffraction pattern of this material to measure z for the Cd and the Au.

4) The structure of KAlF_4 is given in the Table, below.

- (i) 5% Sketch this structure projected down the [010] axis.
- (ii) 10% Determine the Al-F bond length and describe the polyhedron formed by the Al and F.
- (iii) 10% Describe how the AlF_n polyhedra are connected in the structure and sketch this arrangement.

Table 1: The Structure of potassium aluminum fluoride, KAlF₄

Formula unit	KAlF ₄
Space group:	P4/mmm (no. 123)
Cell dimensions:	a = 3.350 Å c = 6.139 Å
Cell contents:	1 formula units per cell
Atomic positions:	K in 1a 0,0,0
	Al in 1d 1/2,1/2,1/2
	F(1) in 2e 0,1/2,1/2; 1/2,0,1/2
	F(2) in 2h 1/2,1/2,z; 1/2,1/2,□
	z = 0.21

5) The following questions are about the AO₂ structure. The structural data are in the table below.

- In the compound AO₂, what are the systematic absences caused by the I operator?
- In the compound AO₂, what are the systematic absences caused by the 4₁ operator?
- In the compound AO₂, what are the systematic absences caused by the *a* operator?
- How would one use a diffraction experiment to measure the unknown coordinate, *z*?
- Index the powder diffraction pattern illustrated in Fig the figure below. (in other words, specify the h,k, and l for each of the peaks)

Formula unit	AO ₂
Space group:	I4 ₁ /amd (no. 141)
Cell dimensions:	a = 3.785 Å c = 9.514
Cell contents:	4 formula units
Atomic positions:	A in (4a) 0,0,0; 0, 1/2, 1/4; + I
	O in (8e) 0,0,z; 0,0, \bar{z} ;
	0,1/2,z+1/4; 0,1/2,1/4-z; + I

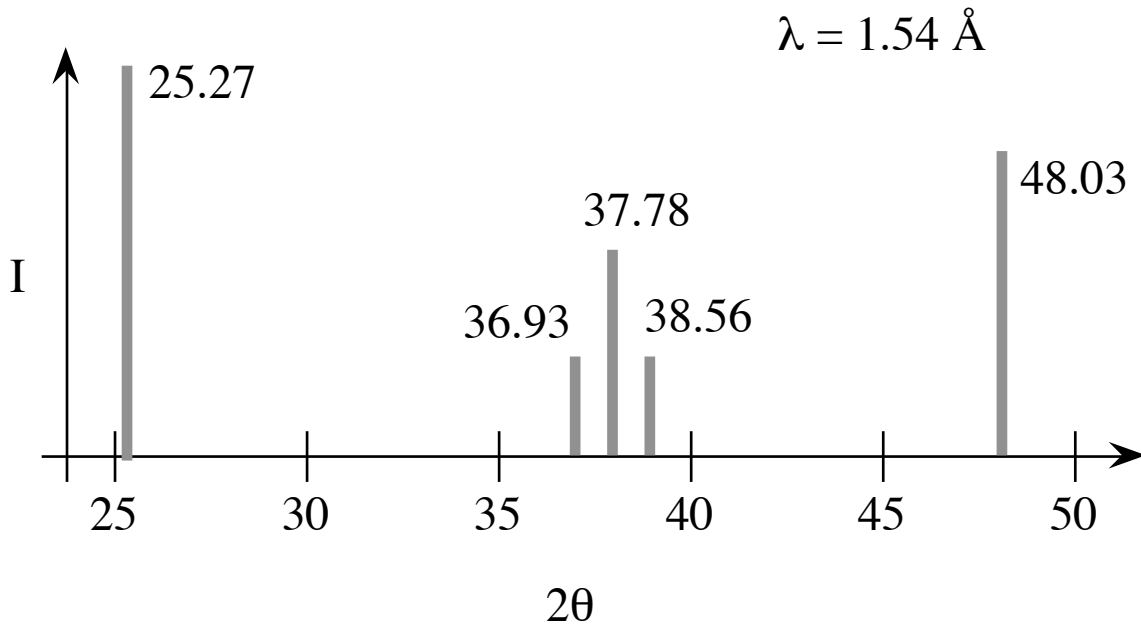


Fig. for problem 5. The relative intensities and positions of diffraction peaks in the powder diffraction pattern of the compound AO_2 . There are possible errors of $\pm 0.1^\circ$.

6) Consider the space group, Pnma .

- (i) What is the Bravais lattice for structures in this group?
- (ii) From what point group does this space group arise?
- (iii) What are the general coordinates in this point group?
- (iv) Explain the meaning of n , its location, and its action on the pattern.
- (v) Explain the meaning of m , its location, and its action on the pattern.
- (vi) Explain the meaning of a , its location, and its action on the pattern.
- (vii) Assuming lattice parameters of 5.453 \AA , 7.672 \AA , 5.447 \AA , sketch projections of the real space lattice and the reciprocal lattice, side by side, projected down the $[001]$ direction. Label the vectors.
- (viii) What is the angle between $[101]$ and the reciprocal lattice vector G_{101} ?

The structure of AB_2

Formula unit	AB_2
Space group:	I4/mmm (no. 139)
Cell dimensions:	$a = 3.00 \text{ \AA}$ $c = 8.65 \text{ \AA}$
Cell contents:	2 formula units per cell
Atomic positions:	B in 4e $0,0,z$ <input type="text"/>
	$z = 0.32$
	A in 2a $0,0,0$

7) Use the data in the table above to answer the following questions:

- (i) What is the Bravais lattice of this structure and what are the coordinates of the lattice points in each cell?
- (ii) What is the basis of this structure?

(iii) Draw the pattern produced by the point group from which this structure is derived, and list the general equivalent coordinates.

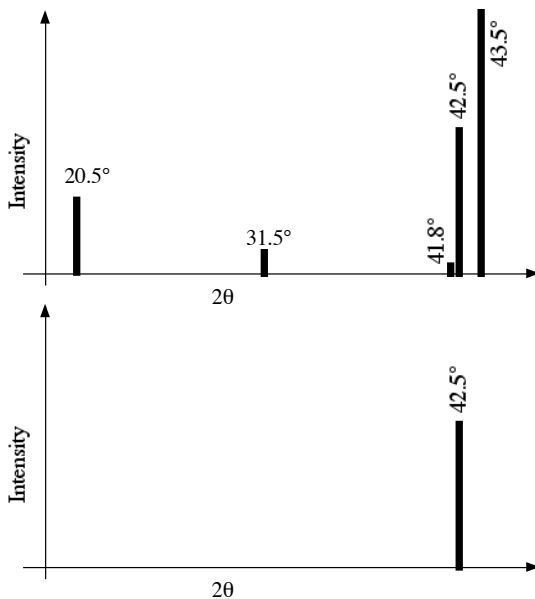
(iv) How many general equivalent positions are there in the space group, $I4/mmm$

8) The table above describes the structure of the compound phase AB_2 at room temperature. At a higher temperature, a disordered cubic phase forms in which the A and B atoms occupy each site with equal probability. The lattice constant for this cubic phase is 3.0 \AA .

(i) There are two schematic powder diffraction patterns shown below. Each was recorded using $\text{Cu K}\alpha$ radiation ($\lambda = 1.54 \text{ \AA}$). One is of the low temperature phase and the other is for the high temperature phase. Determine which pattern corresponds to which phase and index (assign and hkl to) each of the diffraction peaks.

(ii) According to the data in the table above, the value of the parameter "z" was measured to be 0.32. Explain how one can use X-ray diffraction data to determine the coordinate. Include all appropriate equations.

(iii) Between the fully ordered low temperature structure and the completely disordered high temperature structure, there exists a continuous range of partially ordered structural states. Explain how you can use the X-ray diffraction intensity data to measure the degree of order in the structure (this amounts to determining the probability that an A atom is on an A-type site).



9) Interstitial carbides are compounds of certain transition metals and carbon. These compounds combine some of the characteristic properties of metals (luster, high electronic conductivity) with extraordinary hardness. These compounds are often given the general formula MC_x , where x can be any number between 0 and 1. We will assume that in all cases the M atoms occupy the sites of a fcc lattice and that the C atoms occupy octahedral interstices. Please note the following: at the low C concentration limit ($x=0$) this is simply an fcc metal and at the high C concentration limit ($x=1$) all of the octahedral sites are filled and thus, the structure of MC is rock salt. To answer the

following questions, assume that the volume of the unit cell is constant with x and that when x takes fractional values (neither 0 nor 1) the available octahedral sites are randomly occupied.

- (i) Explain why Ti, V, Zr, Nb, Mo, Hf, Ta, and W all form "interstitial carbides", as described above, but Cr, Fe, Co, and Ni do not (these last four do react to form carbides, but with more complex structures).
- (ii) Explain how you could use X-ray diffraction measurements to determine the value of x in MC_x . Your explanation must be quantitative. In other words, it should include the appropriate equations that relate interstitial occupation to experimental observations.
- (iii) Would the accuracy of your method be the same for all of the interstitial carbide forming metals (Ti, V, Zr, Nb, Mo, Hf, Ta, and W) ?