Solutions

PHY 481/581 - HOMEWORK SET 4

Northern Arizona University   Due: 11/05/2018

Problem 1. Determine the Miller indices of the four sets of planes in Fig.1 for **both** coordinate systems a and b.

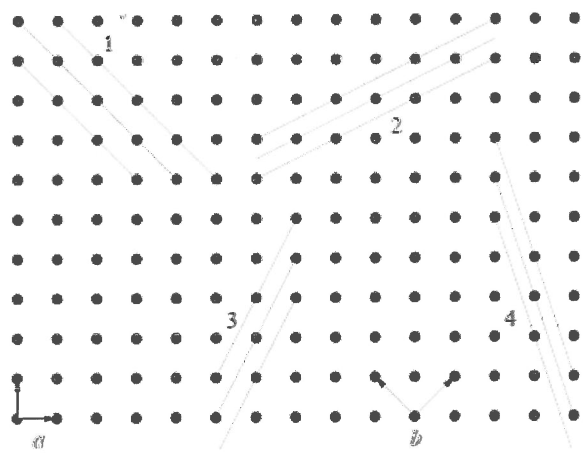


Figure 1: Lattice planes for the square lattice. Coordinate systems a and b are defined at the bottom.

Problem 2. Determine which planes in an FCC structure have the highest density of atoms and evaluate this density for Cu, where the inter-atomic spacing is $a = 3.61 \times 10^{-10}$m.

Problem 3. Reciprocal lattice:

(a) Calculate the primitive translation vectors of the reciprocal lattice for a simple cubic (SC) lattice with the cube edge a and determine the Bravais lattice of the reciprocal lattice.

(b) Do the same thing for a BCC lattice with the cube edge a.

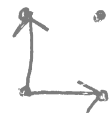
(c) Do the same thing for an FCC lattice with the cube edge a.

Problem 4. From an X-ray diffraction experiment on NaCl, diamond, and CsCl crystal types, determine which sample is which from the following results:

Bragg angle	Sample 1	Sample 2	Sample 3
θ_1	10.8°	13.7°	22.0°
θ_2	15.3°	15.9°	37.7°
θ_3	18.9°	22.8°	45.8°
θ_4	22.0°	27.0°	59.8°
θ_5	24.7°	28.3°	70.4°

(1)

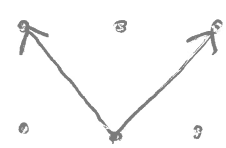
- for coordinate system 'a'



- families of planes (Fig. 1) Miller indicies

families of planes (Fig. 1)	Miller indicies
1	$(1\ 1\ 0)$
2	$(1\ \bar{2}\ 0)$
3	$(2\ \bar{1}\ 0)$
4	$(3\ 1\ 0)$

- for coordinate system 'b'



families of planes	Miller indicies
1	$(2\ 0\ 0)$
2	$(1\ 3\ 0)$
3	$(\bar{1}\ 3\ 0)$
4	$(4\ \bar{2}\ 0)$

(2) the {1 1 1} planes have the highest density for FCC.

For Cu with interatomic spacing

$$a = 3.61 \times 10^{-10} m$$

this density is

$$\rho = \frac{2\sqrt{12}}{3a^2} \approx 0.177 \times 10^{20} \frac{\text{atoms}}{m^2}$$

(3) Start by finding the primitive lattice vectors

(a) for the simple cubic

$$\vec{a}_1 = a\hat{x}$$
$$\vec{a}_2 = a\hat{y}$$
$$\vec{a}_3 = a\hat{z}$$

- Use the following relation to find the first reciprocal lattice vector, $\vec{b}_1$

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_1}$$

$$= \frac{2\pi}{a^2} a\hat{x} = \frac{2\pi}{a}\hat{x}$$

- for $\vec{b}_2$ + $\vec{b}_3$, we have similar relations giving

$$\vec{b}_2 = \frac{2\pi}{a}\hat{y} \quad \& \quad \vec{b}_3 = \frac{2\pi}{a}\hat{z}$$

- a SC lattice with lattice constant $2\pi/a$

(3)

(b) the direct lattice vectors for BCC

$$\vec{a}_1 = \frac{1}{2}a(-\hat{x}+\hat{y}+\hat{z})$$

$$\vec{a}_2 = \frac{1}{2}a(\hat{x}-\hat{y}+\hat{z})$$

$$\vec{a}_3 = \frac{1}{2}a(\hat{x}+\hat{y}-\hat{z})$$

- which gives

$$\vec{b}_1 = \frac{2\pi}{a}(\hat{y}+\hat{z})$$

$$\vec{b}_2 = \frac{2\pi}{a}(\hat{x}+\hat{z})$$

$$\vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y})$$

} FCC with lattice constant $4\pi/a$

(c) for the FCC

$$\vec{a}_1 = \frac{1}{2}a(\hat{y}+\hat{z})$$

$$\vec{a}_2 = \frac{1}{2}a(\hat{x}+\hat{z})$$

$$\vec{a}_3 = \frac{1}{2}a(\hat{x}+\hat{y})$$

$$\vec{b}_1 = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z})$$

$$\vec{b}_2 = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z})$$

$$\vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z})$$

} BCC with lattice const. $4\pi/a$

④ Start with selection rules

Chemical	Structure	Selection rules
NaCl	FCC	all h,k,l even or all h,k,l odd
CsCl	SC	all h,k,l
diamond	diamond	all h,k,l even, h+k+l=4n all h,k,l odd

• take the square of Bragg's law

$$\sin^2\theta = \frac{\lambda^2}{2^2 a^2}\underbrace{(h^2+k^2+l^2)}_{N}$$

Sample 1

θ	$\frac{\sin^2\theta}{\sin^2\theta_0}$	N	(hkl)
10.8°	1	1	100
15.3°	2	2	110
18.9°	3	3	111
22.0°	4	4	200
24.7°	5	5	210

Sample 2

θ	$\frac{\sin^2\theta}{\sin^2\theta_0}$	N	{hkl}
13.7°	1	3	111
15.9°	4/3	4	200
22.8°	8/3	8	220
27.0°	11/3	11	311
28.3°	12/3	12	222

→ over

#4 continued

Sample 3

Θ	$\frac{\sin^2\Theta}{\sin^2\Theta_0}$	N	{hkl}
22.0°	1	3	111
37.7°	8/3	8	220
45.8°	11/3	11	311
59.8°	16/3	16	400
70.4°	19/3	19	331

- comparing to the selection rules,

Sample 1 → CsCl

Sample 2 → NaCl

Sample 3 → diamond