HOMEWORK OF SURFACE PHYSICS

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1. For Si crystal, find the 2θ value and relative intensities for the first 5 existing diffraction peaks in powder XRD, assume X-ray wavelength of 0.5Å.

Proof. We could get the structure of Si is FCC with two basis at (000) and $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ from *Springer Materials* with lattice parameters $a = 5.43$Å. There are 8 atoms in each unit cell and the relative positions of atoms are

$$\vec{r}_0 = (0,0,0);\ \vec{r}_1 = (1/4,1/4,1/4);\ \vec{r}_2 = (1/2,1/2,0);\ \vec{r}_3 = (3/4,3/4,1/4);$$

$$\vec{r}_4 = (1/2,0,1/2);\ \vec{r}_5 = (3/4,1/4,3/4);\ \vec{r}_6 = (0,1/2,1/2);\ \vec{r}_7 = (1/4,3/4,3/4).$$

The vector basis are

$$\vec{a}_1 = a(1,0,0);\ \vec{a}_2 = a(0,1,0);\ \vec{a}_3 = a(0,0,1).$$

Then we could determine the volume of an unit cell

$$V = \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 = a^3.$$

The reciprocal basis are

$$\vec{b}_1 = \frac{2\pi}{a}(1,0,0);\ \vec{b}_2 = \frac{2\pi}{a}(0,1,0);\ \vec{b}_3 = \frac{2\pi}{a}(0,0,1).$$

Then we could determine the structure factor as below

$$\begin{aligned} F =& \sum_{j=0}^{7} f_j e^{-i\vec{G}_{hkl}\cdot\vec{r}_j} = f\sum_{j=0}^{7} e^{-i\vec{G}_{hkl}\cdot\vec{r}_j} \\ =& f\left(1+e^{-i\frac{\pi}{2}(h+k+l)}\right)\left(1+e^{-i\pi(h+k)}+e^{-i\pi(h+l)}+e^{-i\pi(k+l)}\right). \end{aligned}$$

The conditions for $F = 0$ are that h, k, l are all even or all odd or $\frac{h+k+l}{2}$ is odd.
The interplanar crystal spacing with Miller indices (hkl) is

$$d_{hkl} = \frac{2\pi}{|\vec{G}_{hkl}|} = \frac{a}{\sqrt{h^2+k^2+l^2}}.$$

Then we could determine the five least interplanar crystal spacing and multiplicity factor $M(h,k,l)$ are

hkl	111	220	311	400	331
d_{hkl}/Å	3.14	1.92	1.64	1.36	1.25
$M(hkl)$	8	12	24	6	24

Utilizing the Bragg's diffraction formula

$$2d\sin\theta = n\lambda,$$

we could determine the diffraction angles for different n and different indices as below

hkl	111	220	311	400	331
d_{hkl}/Å	3.14	1.92	1.64	1.36	1.25
$\theta = \arcsin\frac{\lambda}{2d}$	4.57	7.48	8.77	10.59	11.54
2θ	9.14	14.96	17.54	21.19	23.07

Then we could get the five smallest angles and the number of equivalent indices for each diffraction theta m are

θ	4.57	7.48	8.77	10.59	11.54
2θ	9.14	14.96	17.54	21.19	23.07
$M(hkl)$	8	12	24	6	24

Utilizing the formula

$$I_{hkl} \propto M(h,k,l) \times |F(h,k,l)|^2 \times \frac{1+\cos^2(2\theta)}{\sin^2\theta\cos\theta},$$

the relative intensity for each d_{hkl} with corresponding value of θ is

hkl	111	220	311	400	331
θ	4.57	7.48	8.77	10.59	11.54
2θ	9.14	14.96	17.54	21.19	23.07
$M(hkl)$	8	12	24	6	24
$F(h,k,l)$	$4(1+i)f$	$8f$	$4(1-i)f$	$8f$	$4(1+i)f$
$\lvert F\rvert^2/\lvert f\rvert^2$	32	64	32	64	32
I_{hkl}/I_{max}	0.90	1	0.72	0.24	0.41

□

2. An element, BCC or FCC, shows diffraction peaks at 2θ of $40, 58, 73, 86.8, 100.4$ and 114.7 (with X-ray wavelength of 1.54Å). Determine: (a) Crystal structure? (b) Lattice constant? (c) What is the element?

Proof. (a) According to the Bragg's diffraction formula

$$2d\sin\theta_i = n_i\lambda,$$

we could get the table as below.

2θ	40	58	73	86.8	100.4	114.7
θ	20	29	36.5	43.4	50.2	57.35
$d = \frac{\lambda}{2\sin\theta}$	2.25	1.59	1.29	1.12	1.00	0.91
$(d_{max}/d)^2$	1.00	2.00	3.04	4.04	5.06	6.06

Since $N = h^2 + k^2 + l^2 = 1$ is not allowed for neither FCC nor BCC, we need to consider the integral multiple of $(d_{max}/d)^2$.

If we consider $2(d_{max}/d)^2$, we could get the table as below

$2(d_{max}/d)^2$	2	4	6	8	10	12
(hkl)	(110)	(200)	(211)	(220)	(310)	(222)

It is clearly that $h + k + l$ is even, which shows that the crystal structure could be BCC.

If we consider $3(d_{max}/d)^2$, we could get the table as below

$3(d_{max}/d)^2$	3	6	9	12	15	18
(hkl)	(111)	(211)	(300)/(221)	(222)	none	(330)

Since (211) is forbidden for FCC, the crystal structure could not be FCC.

Thus, the crystal structure is BCC.

(b) The lattice constant a satisfy

$$d_{max} = \frac{a}{\sqrt{1^2 + 1^2 + 0^2}} = \frac{a}{\sqrt{2}}.$$

So the lattice constant is $a = 3.18$Å.

(c) Compared with the database, we could get the element could be W (a=3.16Å) or Mo (a=3.15Å)

□