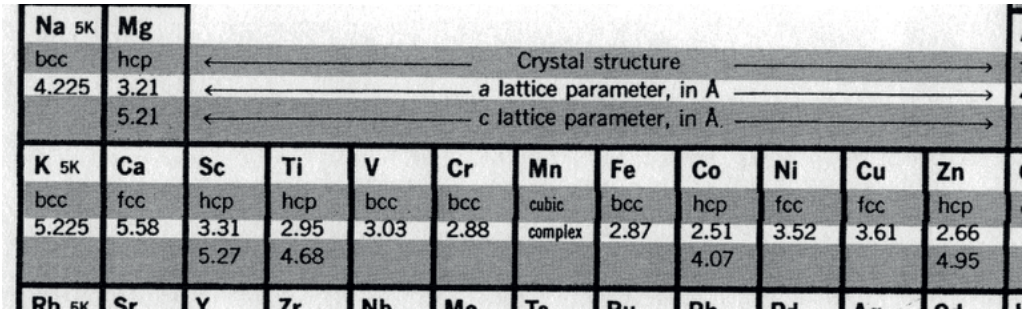
Condensed Matter Physics: Weekly Problem 2

These problems are to be formatively self-assessed by you, the student. Students taking part in the peer-marking pilot scheme will also be required to mark one of their peer's weekly problems. A mark scheme, out of 10, will be provided with each solution to aid your assessment before your timetabled weekly workshop. Information underlined/boxed in red in the model solutions is required for marks to awarded.

Summary: X-ray diffraction measurements from powdered samples give a precise determination of lattice constant and also confirm the crystal structure. Consider the following extract from the periodic table taken from Kittel Chapter 1 Table 3 (page 20).



Na 5K	Mg	← Crystal structure →									
bcc	hcp										
4.225	3.21	← a lattice parameter, in Å →									
	5.21	← c lattice parameter, in Å →									
K 5K	**Ca**	**Sc**	**Ti**	**V**	**Cr**	**Mn**	**Fe**	**Co**	**Ni**	**Cu**	**Zn**
bcc	fcc	hcp	hcp	bcc	bcc	cubic	bcc	hcp	fcc	fcc	hcp
5.225	5.58	3.31	2.95	3.03	2.88	complex	2.87	2.51	3.52	3.61	2.66
		5.27	4.68					4.07			4.95

a. Starting with the structure factor relationship, given in lectures, and by considering the position of the unique atoms within the unit cell of a lattice having the same structure as calcium (Ca), obtain the structure factor rules for this lattice. **[3 marks]**

b. For an incident x-ray beam of wavelength 0.15 nm, calculate the scattering angles 2θ for the first four observed peaks in an x-ray power diffraction measurement of calcium. Determine the Miller indices of these four peaks. **[4 marks]**

c. Explain why there is no peak observed for diffraction from the (100) planes. **[1 mark]**

d. Without doing any calculations describe qualitatively what the difference would be if calcium were replaced by copper (Cu). Explain your reasoning. **[2 marks]**

Condensed Matter Physics: Weekly Problem 2 - Solutions

When completing your assessment please enter the numerical marks for each question. Please also give information on any parts which you found difficult, as this will allow me to go over any common issues in the workshops. The workshops also provide the opportunity to individually talk to myself, and other staff members about any issues you faced when solving the problem. Information in the model solutions underlined/boxed in red is required for marks to awarded.

a. The structure factor describes the intensity pattern of scattered x-rays from a crystal, given by:

$$S(h,k,l) = \sum_{\text{cell}} f \exp\left[-2\pi i\left(hx_j + ky_j + lz_j\right)\right]$$

where the summation is performed over the unit cell. The *hkl* values are the relevant Miller indices, the *xyz* values are the position coordinates of the atoms in the unit cell with respect to the origin. The summation is performed over all the unique atoms in the unit cell (subscript *j*). The *f* is the atomic form factor which determines the intensity of the scattered radiation from a single atom and is related to the atomic number *z*. **[1 mark]**

Calcium has the fcc structure so you need to do the structure factor calculations for the fcc lattice. The fcc basis has atoms at the following 4 coordinates in the unit cell: (0 0 0), (0 ½ ½), (½ 0 ½) and (½ ½ 0). **[1 mark]**

Substituting (*x,y,z*) for each of the four coordinates above and doing the summation gives:

$$S(h,k,l) = f[\exp 0 + \exp i\pi(k+l) + \exp i\pi(h+l) + \exp i\pi(h+k)]$$

We can use the relation to show that:

- $S(h,k,l) = 4f$ when *h k* and *l* are either all odd or all even.
- $S(h,k,l) = 0$ when *h k* and *l* are of mixed parity. **[1 mark]**

b. These two rules allow us to determine which values of h k l and therefore N should be present for a fcc structure. The possible hkl values are obtained from $N = h^2 + k^2 + l^2$.

[1 mark]

N	Possible h k l	Indices	Peak Present?
1	1 0 0	Mixed	No
2	1 1 0	Mixed	No
3	***1 1 1***	***All Odd***	***Peak 1***
4	***2 0 0***	***All Even***	***Peak 2***
5	2 1 0	Mixed	No
6	2 1 1	Mixed	No
8	***2 2 0***	***All Even***	***Peak 3***
9	2 2 1 / 3 0 0	Mixed	No
10	3 1 0	Mixed	No
11	***3 1 1***	***All Odd***	***Peak 4***

[1 mark]

(Remember that $N = 7$ does not exist, and a zero is treated as even).

For a cubic lattice: $$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{a}{\sqrt{N}}$$

Using Bragg's Law and rearranging the above gives: $\sin\theta = \lambda\sqrt{N}/\ 2a$ **[1 mark]**

(Here we have made use of Bragg's Law of diffraction: $2d \sin\theta = n\lambda$*).*

Using the data, we can tabulate values for N to determine the values of: d, $\sin\theta$ and thus 2θ:

Peak	N	d (nm)	sinθ	θ	2θ
1	3	0.3222	0.2328	13.46	26.92
2	4	0.2790	0.2688	15.59	31.19
3	8	0.1973	0.3802	22.34	44.69
4	11	0.1682	0.4458	26.47	52.95

[1 mark]

c. For subsequent (100) planes in an fcc lattice the phase difference between reflections from adjacent planes is π. The reflected amplitude from two adjacent planes is therefore: $1 + \exp(-i\pi) = 0$. **[1 mark]**

(See Kittel page 41, Figure 16 for more detail on this point).

d. Copper has a much smaller lattice constant a therefore the equivalent planes will be spaced closer together with smaller d. This in turn will significantly increase the angle at which the x-ray peaks are observed. **[1 mark]**

Copper also has the same fcc structure so would you see the same N values with the same structure factor rules. **[1 mark]**