Introduction to Condensed Matter Physics Assignment

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Note: References to materials presented in the lecture notes will be denoted with [LN-n], where N is the lecture number and n is the slide number. The computation and analysis in Question 1 is done using a Python script written specifically for this problem. Questions 2 and 3 are hand-written.

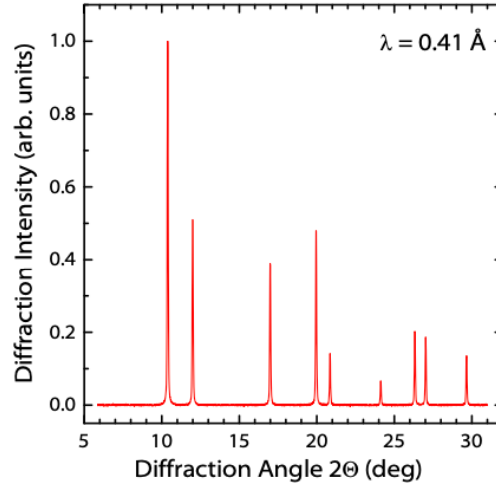## 1 Indexing a Powder Diffraction Pattern

Figure 1: Given diffraction intensity data.

a) Calculate the d-spacings (interplanar spacings) for these 9 reflections.

We begin by quoting Bragg's Law [L2-18]

$$2d_{hkl}\sin\theta = \lambda \tag{1}$$

where d_{hkl} is the interplanar spacing corresponding to the (hkl) plane, 2θ the diffraction angle and λ is the radiation wavelength used to probe the material. Trivially, we invert Equation 1 to yield the corresponding d_{hkl} in Figure 2.

The values in 3 s.f. with the correct units is given in Table 1 for completeness.

	0	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
$d_{hkl}(\mathring{A})$	2.27	1.96	1.39	1.18	1.13	0.981	0.900	0.878	0.801

Table 1: The top row identifies the diffraction angle corresponding to the calculated d_{hkl}, which can be matched with the data in Figure 2.

1

	Diffraction angle	d_hkl
0	10.378	2.266662
1	11.992	1.962492
2	16.999	1.387002
3	19.955	1.183183
4	20.858	1.132491
5	24.118	0.981242
6	26.332	0.900018
7	27.019	0.877544
8	29.661	0.800905

Figure 2: The calculated value of interplanar spacing d_{hkl} in units of $\mathring{A}$.

b) Using the expression for the interplanar spacings in a cubic crystal, assign Miller indices (hkl) to each of the 9 observations. Is your solution the only viable solution, or are there alternatives that explain the observed pattern equally well? Document which alternative candidates you have excluded and why. As explained in the lectures, this is inherently a trial-and-error process, but proceed methodically and remember that there may be systematic absences.

We proceed by assuming the hint given in the question, which is to use the interplanar spacing formula for a *cubic* crystal given by [L3-10]

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}, \tag{2}$$

where a is the lattice parameter and h, k, l are the Miller indices, and we can rearrange this into

$$a = d_{hkl} \underbrace{\sqrt{h^2 + k^2 + l^2}}_{g_{hkl}} \tag{3}$$

where we have defined the square root of the square sum factor as g_{hkl} to ease notation. This greatly reduces the search to either a *bcc* or *fcc* crystal. The general strategy that we are adopting is to work out all possible h, k, l combinations for each d_{hkl} and find the values for which the lattice parameter a remains *approximately* constant. Recall from [L4-8] the systematic absences for the two crystal structures:

bcc Intensities are only visible for even $h + k + l$

fcc Intensities are only visible for h, k, l all odd or even.

One crucial observation is to realise that Equation 3 implies that $d_{hkl} \propto \frac{1}{g_{hkl}}$; that is to say that if we order d_{hkl} in a decreasing manner, the corresponding h_{hkl} values should increase (†)[1].

In the algorithm used for the trial and error process, the integers h, k, l are each capped at 4 to calculate the values of a for each d_{hkl}, considering only the *unique families* of Miller indices to avoid degeneracies. The (0 0 0) index and indices corresponding to systematic absences are discarded, and the Miller indices (hkl) are ordered by increasing g_{hkl}. Since the data provides diffraction angles for the first nine reflections, it is reasonable to only take the data for the nine smallest g_{hkl}.

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[1]This statement is marked with a dagger due to its importance for our calculation, and we will refer to this again

g_hkl	d=2.2666150436235 5	d=1.9624918545794 45	d=1.3870021493727 2716	d=1.1831831157994 568	d=1.1324906166151 893	d=0.9812423684906 892	d=0.9000184967882 933	d=0.8775437533120 479	d=0.8009051826097 932
(1, 1, 1) 1.732051	3.925973	3.399136	2.402358	2.049333	1.961531	1.699562	1.558878	1.519950	1.387208
(0, 0, 2) 2.000000	4.533323	3.924984	2.774004	2.366366	2.264981	1.800037	1.800037	1.755088	1.601810
(0, 2, 2) 2.828427	6.411087	5.550765	3.923035	3.346547	3.203167	2.775373	2.545637	2.482069	2.265302
(1, 1, 3) 3.316625	7.517666	6.508849	4.600166	3.924174	3.756046	3.254413	2.985024	2.910483	2.656302
(2, 2, 2) 3.464102	7.851946	6.798271	4.804716	4.098667	3.923063	3.399123	3.117756	3.039901	2.774417
(0, 0, 4) 4.000000	9.066646	7.849967	5.548009	4.732732	4.529962	3.924969	3.600074	3.510175	3.203621
(1, 3, 3) 4.358899	9.880148	8.554304	6.045802	5.157376	4.936412	4.277136	3.923090	3.825125	3.491065
(0, 2, 4) 4.472136	10.136818	8.776530	6.202862	5.291356	5.064652	4.388249	4.025005	3.924495	3.581757
(2, 2, 4) 4.898979	11.104328	9.614207	6.794895	5.796390	5.548048	4.807086	4.409172	4.299069	3.923618

Figure 3: The calculated values for *fcc* crystal. First column denotes the Miller indices. The *d* values in the top row is in Å and the nine columns on the right are all the possible *a* values for each combination of *d* and (*hkl*).

g_hkl	d=2.2666150436235 5	d=1.9624918545794 45	d=1.3870021493727 2716	d=1.1831831157994 568	d=1.1324906166151 893	d=0.9812423684906 892	d=0.9000184967882 933	d=0.8775437533120 479	d=0.8009051826097 932
(0, 1, 1) 1.414214	3.205543	2.775383	1.961517	1.673274	1.601584	1.387686	1.272818	1.241034	1.132651
(0, 0, 2) 2.000000	4.533323	3.924984	2.774004	2.366366	2.264981	1.962485	1.800037	1.755088	1.601810
(1, 1, 2) 2.449490	5.552164	4.807104	3.397448	2.898195	2.774024	2.403543	2.204586	2.149534	1.961809
(0, 2, 2) 2.828427	6.411087	5.550765	3.923035	3.346547	3.203167	2.775373	2.545637	2.482069	2.265302
(0, 1, 3) 3.162278	7.167813	6.205944	4.386086	3.741554	3.581250	3.102961	2.846108	2.775037	2.532685
(2, 2, 2) 3.464102	7.851946	6.798271	4.804716	4.098667	3.923063	3.399123	3.117756	3.039901	2.774417
(1, 2, 3) 3.741657	8.481071	7.342972	5.189687	4.427066	4.237392	3.671473	3.367561	3.283468	2.996713
(0, 0, 4) 4.000000	9.066646	7.849967	5.548009	4.732732	4.529962	3.924969	3.600074	3.510175	3.203621
(0, 3, 3) 4.242641	9.616630	8.326148	5.884552	5.019821	4.804751	4.163059	3.818455	3.723103	3.397953

Figure 4: The calculated values for *bcc* crystal. First column denotes the Miller indices. The *d* values in the top row is in Å and the nine columns on the right are all the possible *a* values for each combination of *d* and (*hkl*).

d-spacing (Angstrom)	2.27	1.96	1.39	1.18	1.13	0.981	0.9	0.878	0.801
Miller Indices (hkl)	(1, 1, 1)	(0, 0, 2)	(0, 2, 2)	(1, 1, 3)	(2, 2, 2)	(0, 0, 4)	(1, 3, 3)	(0, 2, 4)	(2, 2, 4)
Lattice Parameter, a (Angstrom)	3.925972889	3.924983709	3.923034501	3.924174453	3.923062574	3.924969474	3.923089675	3.924494971	3.923618059

Figure 5: The assignment of d-spacing to Miller indices (hkl) for fcc crystal structure.

d-spacing (Angstrom)	2.27	1.96	1.39	1.18	1.13	0.981	0.9	0.878	0.801
Miller Indices (hkl)	(0, 1, 1)	(0, 0, 2)	(1, 1, 2)	(0, 2, 2)	(0, 1, 3)	(2, 2, 2)	(1, 2, 3)	(0, 0, 4)	(0, 3, 3)
Lattice Parameter, a (Angstrom)	3.205543441	3.924983709	3.397447538	3.346547218	3.581249777	3.399123274	3.367560857	3.510175013	3.397952914

Figure 6: The assignment of d-spacing to Miller indices (hkl) for bcc crystal structure.

Using statement (†) and the order of the set of diffraction angle, we choose the first (hkl) corresponding to the first diffraction intensity, to be the one with the lowest g_{hkl}. The rest of the intensity-(hkl) correspondence follow suit by picking out the diagonals (underlined) in Figure 3 and Figure 4. The only reason we chose to fix the first intensity with (hkl) of lowest g_{hkl} is because we were given the fact that we have the *first* nine diffraction intensities. Had it been any *consecutive* nine intensities, the constraint is lifted and hence any diagonal can be chosen, granted we extend Figure 3 and Figure 4 to include values for (hkl) of higher g_{hkl}.

For the cubic crystal, we get two possible d-spacing-to-(hkl) assignments, given in Figure 5 (for fcc crystal structure) and Figure 6 (bcc crystal structure). We further calculate the average and uncertainty (as given by the standard deviation) and yield the following results given in Table 2.

	Average Lattice Parameter, a_{av}	Standard Deviation, σ	Uncertainty, σ_m
fcc	3.92415559	0.001039407	0.000346469
bcc	3.458953749	0.203424536	0.067808179

Table 2: The average lattice parameter, standard deviation and the uncertainty.

Finally, we choose to assign the Miller indices using the fcc crystal structure data in Figure 5 as the standard deviation in the calculated lattice parameter is much lower than in the bcc configuration. For clarity, we can match the Miller indices to the corresponding diffraction angle by referring to both Figure 2 and Figure 5.

c)   Determine the lattice parameter of the metal and its uncertainty (error margin) using all available data.

From the previous question, we reached the conclusion that the metal should adopt an fcc crystal structure. We define the uncertainty to be the **standard error of the mean** $\sigma_m = \frac{\sigma}{\sqrt{N}}$ where N is the number of measurements (in this case $N = 9$). Having done the calculation in Table 2, we quote in full the lattice parameter with uncertainty

$$a = 3.9242 \pm 0.0003 \mathring{A}. \tag{4}$$

d)   Try to identify the elemental metal that was studied here. Substantiate your answer.

The metal is **Platinum**. It has an fcc crystal structure and lattice parameter $a = 3.9242\mathring{A}$ [1].

References

[1] *Lattice constants of the elements.* Wolfram Research, Inc. URL: https://periodictable.com/Properties/A/LatticeConstants.html.