

Solid State Physics HW3

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To begin, recall Bragg's Law:

$$n\lambda = 2d \sin(\theta) \quad (1)$$

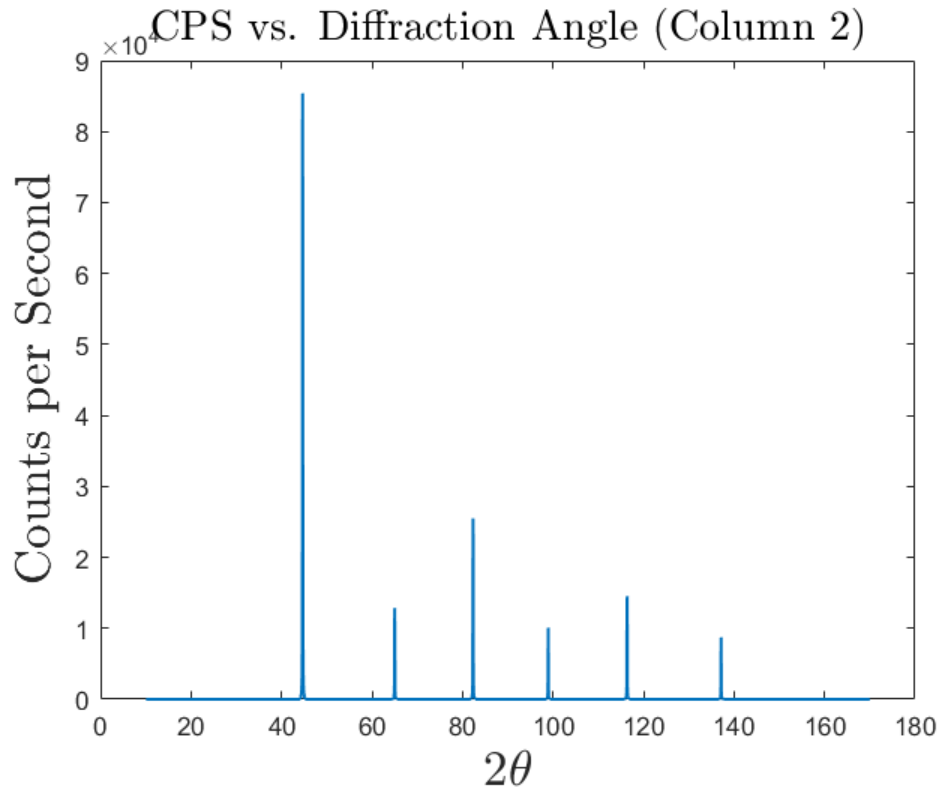
and the formula that relates distance to hkl :

$$d^2 = \frac{a^2}{h^2 + k^2 + l^2} \quad (2)$$

That is, $1/d^2$ is an integer multiple of $1/a^2$, which we may use to solve for a . Additionally, for our use, we will assume $n = 1$ in Bragg's law.

Problem 1

a) Plotting the second column as a function of the first in MATLAB, we find the following plot:



b) After calculating d from Bragg's law for each of the peaks (see table below), we notice that the smallest distance between values of $1/d^2$ is 0.2420903, which leads us to a lattice constant of $a = 2.03241$, with a miller index of the first plane of diffraction of (100), a property that no material possesses. Thus, we must

now consider the case where the first Miller index is (110). As we will see, doing so will lead us to a material that exists.

i	2θ	d [Å]	$1/d^2$ [Å ⁻²]	ratio to 0.1210452	(hkl)
1	44.65°	2.03241	0.2420903	2	(110)
2	65°	1.4368704	0.4843561	4	(200)
3	82.35°	1.17265	0.72721559	6	(211)
4	98.95°	1.01567	0.9693816	8	(220)
5	116.4°	0.908385	1.2118813	10	(310)
6	137.15°	0.82934	1.4539008	12	(222)

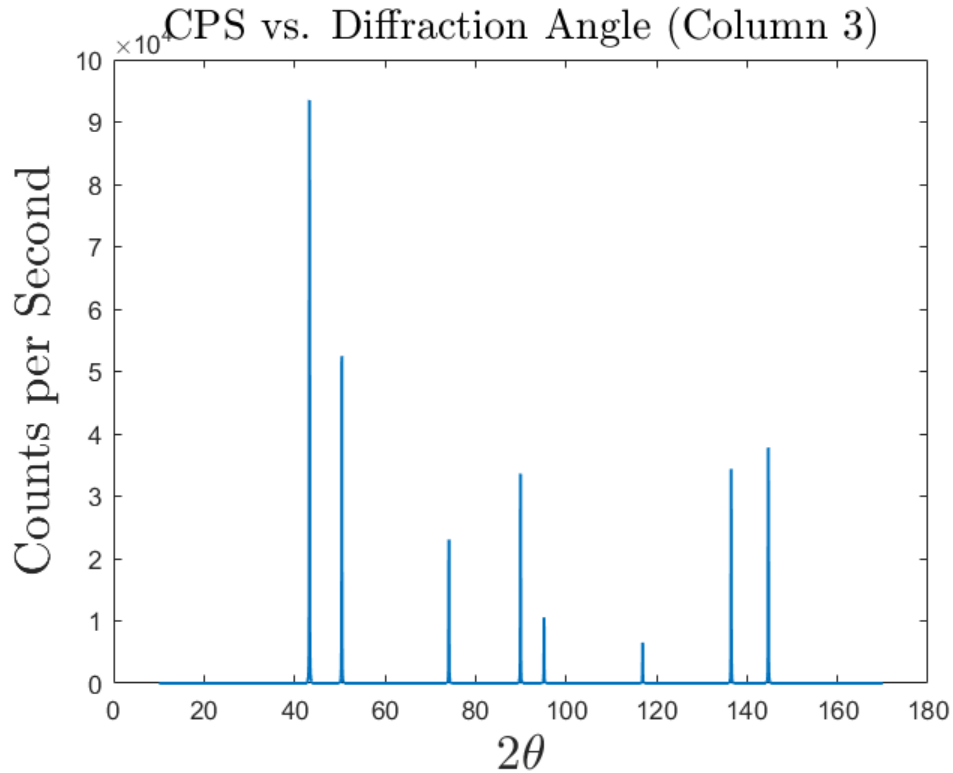
The last column of the above table can be found by solving the Diophantine equation $h_i^2 + k_i^2 + l_i^2 = n_i$, where n denotes the ratio of $1/d^2$ to 0.1210452. Seeing as how the Miller indices are strictly even numbers, it is a fair assumption that this material is in the base centered cubic system.

c) Since the ratio between $1/d_1^2$ and 0.2420903 is two, we can see that the smallest gap between diffraction planes is 0.1210452. Then it is natural to assume $1/a^2 = 0.1210452$ by equation (2), so $a = 2.8743\text{Å}$.

d) Upon inspection of table 3 in Kittel, we can see that iron (Fe) crystallizes in the base centered cubic system and has lattice constant of 2.87Å . Thus, I believe that the most probable material given this data is iron.

Problem 2

e) Plotting the third column as a function of the first, we find



f) Inspecting the peaks of the graphs and using (1) and noticing that the smallest difference between $1/d^2$ terms is 0.076698, we find

i	2θ	d [Å]	$1/d^2$ [Å ⁻²]	ratio to 0.076698	(hkl)
1	43.3°	2.08789	0.229395	3	(111)
2	50.45°	1.80748	0.306093	4	(200)
3	74.15°	1.27774	0.612513	8	(220)
4	89.89°	1.08984	0.841927	11	(311)
5	95.15°	1.04354	0.918294	12	(321)
6	116.95°	0.903670	1.224561	16	(400)
7	136.5°	0.829340	1.453901	19	(331)
8	144.7°	0.808351	1.530383	20	(442)

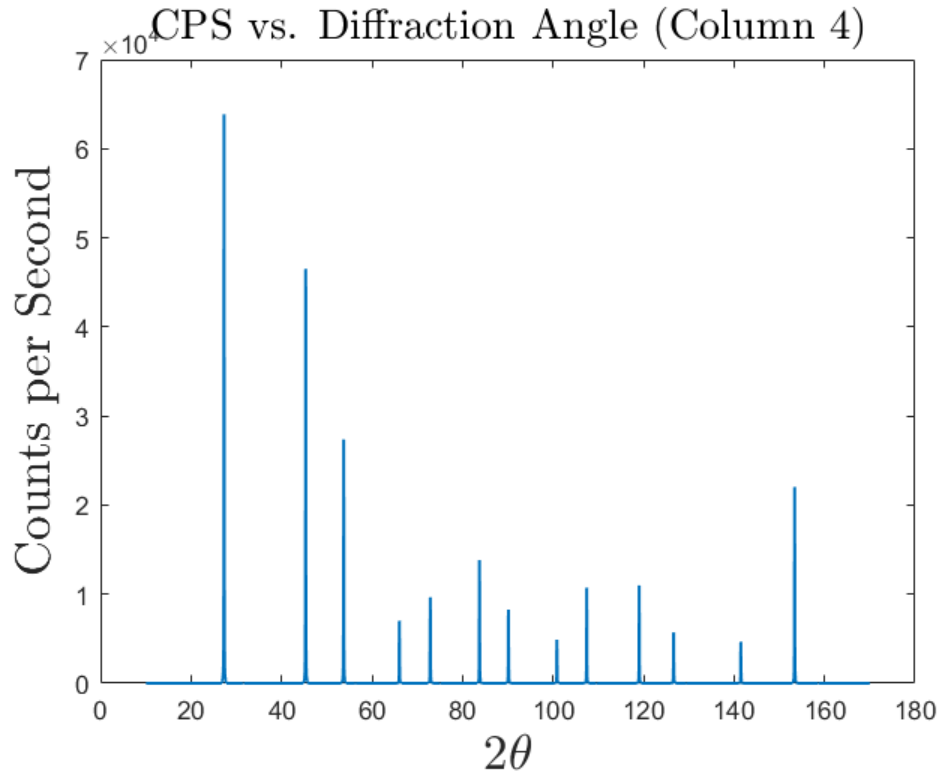
Notice that the Miller indices in the above table satisfy the restrictions for face centered cubic, so it is safe to assume that the material crystallizes in the face centered cubic structure.

g) Since 0.076698 is the smallest difference between values of $1/d^2$, it is natural to assume $1/a^2 = 0.076698$ by equation (2), or alternatively, $a = 3.61084\text{Å}$.

h) Using Table 3 in Kittel, we can see that copper (Cu) is face centered cubic with a lattice parameter of 3.61Å , matching the values we found from this plot. Thus, I believe that Copper is the most probable material given this data.

Problem 3

i) Plotting the fourth column as a function of the first, we find



j) Calculating d by using (1) and noticing that the smallest difference between $1/d^2$ terms is given by 0.0938578, we may also observe that 0.0938578 does not evenly divide into most of the values of $1/d^2$. However, by inspection, it is clear to see that $0.0938578/3 = 0.0312859$ evenly divides each $1/d^2$.

i	2θ	d [Å]	$1/d^2$ [Å ⁻²]	ratio to 0.0312859	(hkl)
1	27.3°	3.26411	0.0938578	3	(111)
2	31.65°	1.26392	0.125329	4	(200)
3	45.35°	1.99816	0.2504606	8	(220)
4	53.75°	1.70403	0.34438603	11	(311)
5	66.05°	1.41338	0.50059	16	(400)
6	72.9°	1.29654	0.594878	19	(331)
7	75.1°	1.26392	0.6359805	20	(420)
8	83.75°	1.15399	0.7509239	24	(422)
9	90.15°	1.08794	0.84487	27	(333)
10	100.85°	0.999361	1.00128	32	(440)
11	107.45°	0.955485	1.095348	35	(531)
12	109.7°	0.942092	1.1267132	36	(600)
13	119.05°	0.893773	1.25183	40	(620)
14	126.65°	0.862049	1.34566	43	(533)
15	129.3°	0.852375	1.376381	44	(622)
16	141.5°	0.815918	1.502128	48	(444)
17	153.4°	0.791529	1.596123	51	(551)

Further notice that the Miller indices satisfy the face centered cubic restrictions, so it is a fair assumption that this substance has face centered cubic structure. Additionally, rows 2, 7, 12, and 15 correspond to peaks with low intensity. Then these bands are essentially "forbidden" and we are working with a compound rather than an element.

k) Seeing as 0.0312859 is the largest divisor for each $1/d^2$ in the above table, it is fair to assume that $1/a^2 = 0.0312859$ by equation (2), or alternatively, $a = 5.65361\text{Å}$

l) On page 18 of Kittel, we can see that gallium arsenide (GaAs) has a lattice parameter of 5.65Å , and happens to be face centered cubic. Thus, I believe that gallium arsenide is the most probable material given this data.

Problem 4

Form factor of atomic hydrogen. For the hydrogen atom in its ground state, the number density is $n(r) = (\pi a_0^3)^{-1} \exp(-2r/a_0)$, where a_0 is the Bohr radius. Show that the form factor is $f_G = \frac{16}{(4+G^2 a_0^2)^2}$.

Proof: Recall the formula for finding the atomic form factor:

$$f_j = 4\pi \int n_j(r) r^2 \sin(Gr) (Gr)^{-1} dr$$

Plugging in the given equation for $n(r)$, our equation becomes

$$f = 4\pi \int_0^\infty r \sin(Gr) e^{-2r/a_0} (\pi a_0^3)^{-1} dr$$

Substituting $x = Gr$ into the above integral gives us

$$f = \frac{4}{G^3 a_0^3} \int_0^\infty x \sin(x) e^{-2x/(Ga_0)} dx$$

Notice the above integral can be rewritten as

$$\frac{4}{G^3 a_0^3} \int x \sin(x) e^{-2x/(Ga_0)} dx = \text{Im} \left\{ \frac{4}{G^3 a_0^3} \int x e^{(i - \frac{2}{Ga_0})x} dx \right\}$$

Solving the right hand side, integration by parts gives us the following:

$$\frac{4}{G^3 a_0^3} \int x e^{\left(i - \frac{2}{G a_0}\right)x} dx = -\frac{2G a_0 + iG^2 a_0^2}{G a_0 i - 2} x e^{-\frac{2}{G a_0} x} [\cos(x) + i \sin(x)] - \frac{(2G a_0 - iG^2 a_0^2)^2}{(4 + G^2 a_0^2)^2} e^{-\frac{2}{G a_0} x} [\cos(x) + i \sin(x)] + C$$

where C is a constant of integration. Using this, we have

$$\operatorname{Im} \left\{ \frac{4}{G^3 a_0^3} \int_0^\infty x e^{\left(i - \frac{2}{G a_0}\right)x} dx \right\} = 4 \left(-\frac{e^{-\frac{2}{G a_0} x}}{4 + G^2 a_0^2} \left[\left(G^2 a_0^2 x - \frac{1}{4 + G^2 a_0^2} 4G^3 a_0^3 \right) \cos(x) + (2G a_0 x + 4G^2 a_0^2) \sin(x) \right] \right) \Big|_0^\infty$$

Evaluating, we find

$$\operatorname{Im} \left\{ \frac{4}{G^3 a_0^3} \int_0^\infty x e^{\left(i - \frac{2}{G a_0}\right)x} dx \right\} = \frac{16}{(4 + G^2 a_0^2)^2}$$

which is what we wanted to show.