X-ray Diffraction - Appendices

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Appendix A: Allowed Reflections for Cubic Lattices

$h^2+k^2+l^2$	Simple Cubic (sc) ***hkl***	Face Centered Cubic (fcc) ***hkl***	Body Centered Cubic (bcc) ***hkl***	Diamond Structure ***hkl***
1	***100***	na	na	na
2	***110***	na	***110***	na
3	***111***	***111***	na	***111***
4	***200***	***200***	***200***	na
5	***210***	na	na	na
6	***211***	na	***211***	na
8	***220***	***220***	***220***	***220***
9	***300 or 221***	na	na	na
10	***310***	na	***310***	na
11	***311***	***311***	na	***311***
12	***222***	***222***	***222***	na
13	***320***	na	na	na
14	***321***	na	***321***	na
16	***400***	***400***	***400***	***400***
17	***410 or 322***	na	na	na
18	***411 or 330***	na	***411 or 330***	na
19	***331***	***331***	na	***331***
20	***420***	***420***	***420***	na
21	***421***	na	na	na
22	***332***	na	***332***	na
24	***422***	***422***	***422***	***422***

Figure 1: Table A1. The hkl, as well as $h^2 + k^2 + l^2$, are given for allowed reflections in four cubic structures. "na" indicates not allowed; there is no reflection for that (hkl) plane.

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Appendix B: Structure Calculation for fcc monatomic material

A monatomic material contains only one type of atom. Thus all atomic positions scatter equally. For a material consisting of several elements (NaCl for example) the calculation of scattering intensities follows the same general idea as presented below, but different "scattering factors" f are used for the two elements - thus the calculation is messier.

For a cubic system, the (hkl) lattice planes, as defined for the Bravais lattice, are separated by a distance

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \tag{1}$$

and the vector

$$\vec{p} = h\hat{x} + k\hat{y} + l\hat{z} \tag{2}$$

is perpendicular to the planes. Thus we can normalize, and find that

$$\vec{d}_{hkl} = \frac{a(h\hat{x} + k\hat{y} + l\hat{z})}{h^2 + k^2 + l^2} \tag{3}$$

is a vector perpendicular to the (hkl) planes of magnitude equal to the spacing between the planes.

For many solids, each lattice point has more than one atom associated with it. The underlying spatial Bravais lattice has each location "decorated" with a several-atom "basis". For the sake of simplicity, consider a two atom basis first.

Since all lattice points in the Bravais lattice are equivalent, we place one Bravais lattice point at the origin, and one atom of the basis is there. The second atom of the basis then is at a location given by

$$\vec{q} = x\hat{x} + y\hat{y} + z\hat{z} \tag{4}$$

which is displaced from the first atom, obviously, by (x, y, z). These second atoms form another identical Bravais lattice displaced from the first atoms' lattice. It is convenient to think of the system, therefore, as one lattice where each lattice point has these two basis atoms associated with it.

The second atom in the basis produces a second set of planes, as shown in Figure 2. What we are concerned with is how the scattered intensity for the reflection from the (hkl) plane may be influenced by the presence of these second atoms/planes.

The distance between the lattice planes formed by the first atom of the basis and those formed by the second atom of the basis is given by

$$L = \frac{g \cdot \vec{d}_{hkl}}{|d|} = \frac{a(xh + yk + zl)}{\sqrt{h^2 + y^2 + l^2}} \tag{5}$$

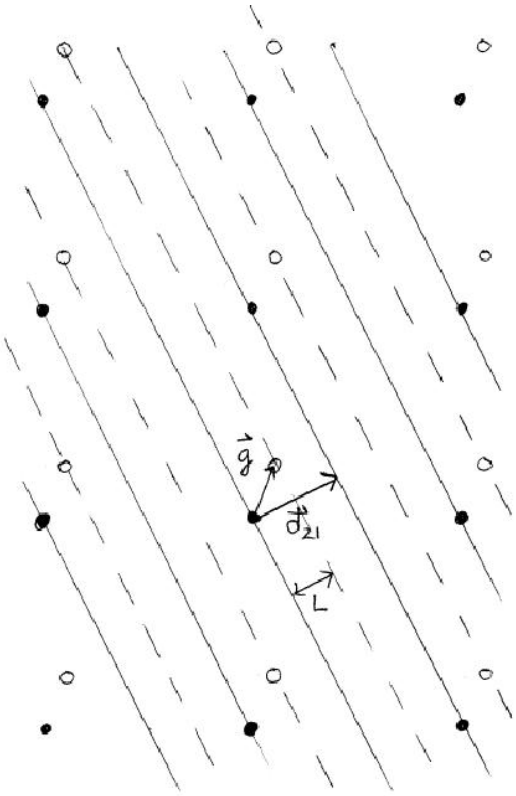

Figure 2: A two dimensional square lattice with a two atom basis. The basis is: • at (0,0) and ◦ at ($1/10$, $1/4$). The (21) planes are shown as solid lines. The dashed lines show the "extra" planes due to the second atom in the basis. The distance L is defined in this Appendix.

The phase difference introduced by the extra path length δ traveled is given by

$$\phi = 2\pi \frac{\delta}{\lambda} \tag{6}$$

where

$$\delta = 2L \sin\theta \tag{7}$$

We already have the Bragg condition satisfied for scattering from the (hkl) planes, that is, we know that

$$\sin\theta = \frac{\lambda}{2a}\sqrt{h^2 + k^2 + l^2} \tag{8}$$

Combining Equations 5, 6, and 8 yields the result:

$$\phi = \frac{2\pi}{a}(xh + yk + zl) \tag{9}$$

Typically we define the fractional distances $u = x/a$, $v = y/a$, $w = z/a$, that is, displacements of the second basis atom are expressed as fractions of the lattice constant. With that, we have the simple result:

$$\phi = 2\pi(uh + vk + wl) \tag{10}$$

This result describes the phase difference for the (hkl) reflection due to the presence of the second basis atom at (uvw).

For a basis with more atoms than just two, we have to add up the scattering from each atom with their individual (uvw) placements.

The scattering factor for an atom is known as f, and using this the wave scattered from an atom with this scattering factor is given by $F = fe^{i\phi}$. For a structure with many atoms, we get the total scattering factor by summing over the different atomic scattering factors f and their positions (uvw). That is, we have

$$F = \sum f_n e^{2\pi(u_n h + v_n k + w_n l)} \tag{11}$$

A face centered cubic structure may be treated as a simple cubic lattice where there are four atoms associated with each lattice point, these are at $(0, 0, 0)$, $(1/2, 1/2, 0)$, $(1/2, 0, 1/2)$ and $(0, 1/2, 1/2)$ where the $1/2$'s are understood to be the distance divided by the simple cubic lattice side a, that is, the (uvw). For the fcc system, then, there are four atoms in the basis (n=4). If all the atoms are identical, their individual structure factors fn are identical. Thus

$$F_{fcc} = f(1 + e^{i\pi(h+k)} + e^{i\pi(h+l)} + e^{i\pi(k+l)}) \tag{12}$$

Where the 1 term is from the atom at the origin since e^0=1. Using Equation 12 , it is trivial to show that some reflections are not allowed, in the sense that their intensity calculated from Equation 12 is zero, which gives the results summarized in Table A1.

For example, Table A1 says the (210) reflection does not exist for an fcc structure. Using h=2, k=1, l=0 in Equation 12 gives

$$F_{210,fcc} = f(1 + e^{i\pi 3} + e^{i\pi 2} + e^{i\pi}) = 0 \tag{13}$$

It is straightforward to evaluate Equation 12 for any (hkl) for an fcc system. For other systems, we must go back to 11 and use the (uvw) for its basis. For a basis with dissimilar atoms, their individual structure factors f_n must be used.