X-ray diffraction and structure factor

Diffracted wave - I

Consider in general the change in the wave vector:

$$\mathbf{\Delta k} = \mathbf{k}' - \mathbf{k}$$

and evaluate the amplitude of the diffracted wave:

Amplitude of diffracted wave

one scattering center on each Bravais lattice point:

$$\mathcal{A} = \sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\mathbf{\Delta k}}$$

Intensity of diffracted wave: $|\mathcal{A}|^2$

Diffracted wave - II

Generalization for a Bravais lattice with basis $\mathbf{d}_j$:

$$\mathcal{A} = \sum_{\mathbf{R}} \sum_{j} f_j(\mathbf{\Delta k}) e^{i(\mathbf{R}+\mathbf{d}_j)\cdot\mathbf{\Delta k}} = \left(\sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\mathbf{\Delta k}} \right) \left(\underbrace{\sum_{j} f_j(\mathbf{\Delta k}) e^{i\mathbf{d}_j\cdot\mathbf{\Delta k}}}_{F(\Delta\mathbf{k})} \right)$$

$$f_j(\mathbf{k}) = \int n(\mathbf{r}) e^{i\mathbf{r}\cdot\mathbf{k}} d\mathbf{r}$$

atomic form factor **crystal structure factor**

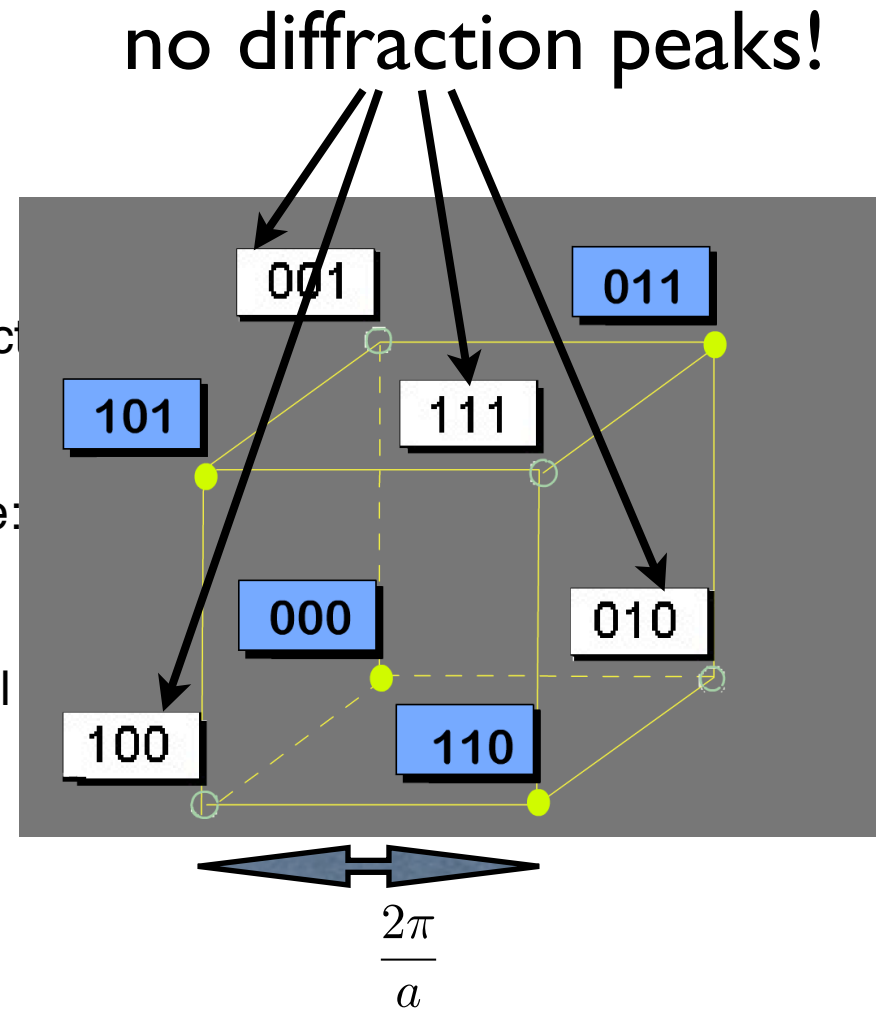
($n(\mathbf{r})$ electron density)

In case of n identical atoms in the basis cell, f_j can be factorized out from $F(\Delta\mathbf{k})$ and in case of Bragg condition ($\Delta\mathbf{k}=\mathbf{K}$), we have the **geometrical structure factor:**

$$S_{\mathbf{K}} = \sum_{j}^{n} e^{i\mathbf{d}_j\cdot\mathbf{K}}$$

BCC structure

considered as a SC with basis



Consider the bcc lattice with single atoms at each lattice point, its unit cell can be reduced to two identical atoms. Atom 1 is at 000 with scattering fact f, and atom 2 is at ½ ½ ½ with a scattering factor f.

The structure factor for the bcc unit cell is therefore:

$$\mathbf{F} = f + f\exp(2\pi\, i(\frac{h}{2}+\frac{k}{2}+\frac{l}{2}))$$
$$= f\,(1+\exp(\pi\, i(h+k+l)))$$

For diffraction from a plane where the sum of h+k+l odd, the second term is -1, so

$F_{hkl\ odd} = f(1-1) = 0$

If h+k+l is even, the second term is +1, so

$F_{hkl\ even} = f(1+1) = 2f$

Thus, diffractions from bcc planes where h+k+l is odd are of zero intensity. They are forbidden reflections. These reflections are usually omitted from the reciprocal lattice.

..drawing a larger reciprocal space cell:

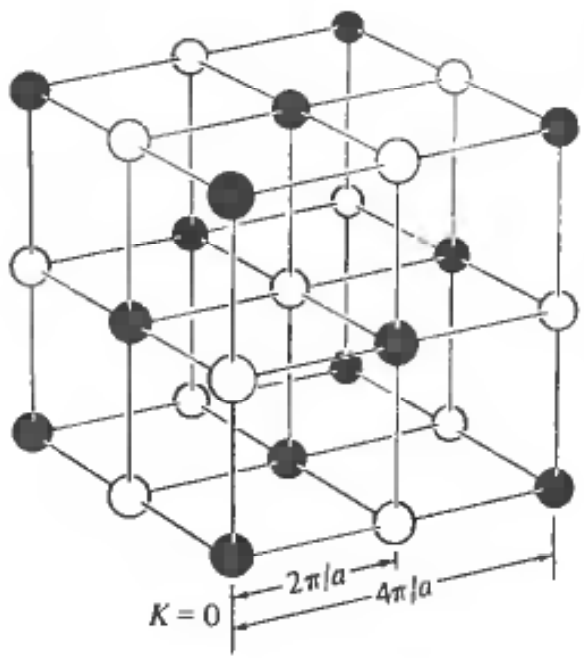


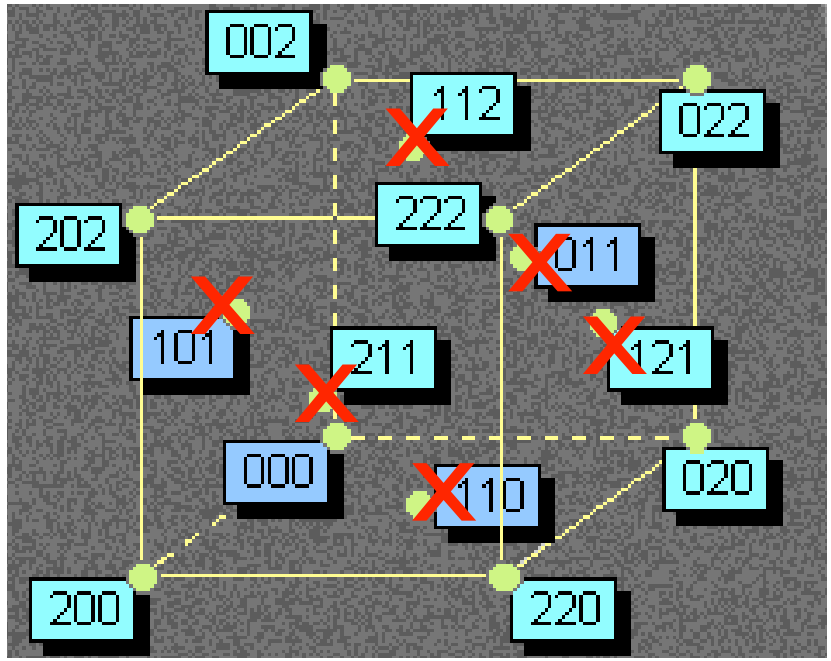
Figure 6.11
Points in the simple cubic reciprocal lattice of side $2\pi/a$, for which the structure factor (6.16) vanishes, are those (white circles) that can be reached from the origin by moving along an odd number of nearest-neighbor bonds. When such sites are eliminated, the remaining sites (black circles) constitute a face-centered cubic lattice with cubic cell of side $4\pi/a$.

Other structures...

Structure factors for other non-primitive structures can be derived similarly. Some important results are:

• forbidden reflections for the **FCC structure** occur when h, k and l are not all even or not all odd (e.g. 211 is forbidden). This time the reciprocal lattice of allowed reflections is bcc with all the indices integer. (Hint: consider again FCC as a SC, now with 4-atoms basis)

• forbidden reflections for the hcp structure occur when h+2k = 3n and l is odd, where n is an integer (e.g. 113 is forbidden).
(DO THE EXERCISE!)



...and also other structures:
DIAMOND as a FCC with basis

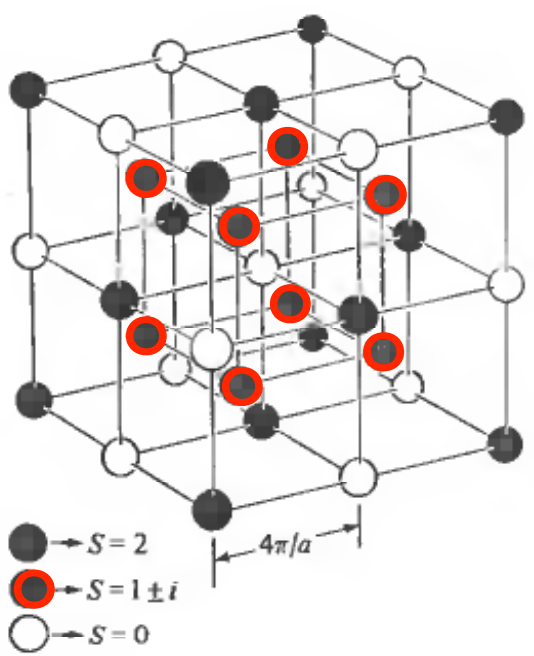


Figure 6.12
The body-centered cubic lattice with cubic cell side $4\pi/a$ that is reciprocal to a face-centered cubic lattice with cubic cell side a. When the fcc lattice is that underlying the diamond structure, then the white circles indicate sites with zero structure factor. (The black circles are sites with structure factor 2, and the gray ones are sites with structure factor $1 \pm i$.)