6 Crystal Structure Methods

Chapter 31

From McQuarrie and Simon (1997).

5/23: **31-26.** Silver crystallizes as a face-centered cubic structure with a unit cell length of 408.6 pm. The single crystal of silver is oriented such that the incident X-rays are perpendicular to the **c** axis of the crystal. The detector is located 29.5 mm from the crystal. What is the distance between the diffraction spots from the 001 and 002 planes on the face of the detector for...

(a) The $\lambda = 154.433$ pm line of copper;

(b) The $\lambda = 70.926$ pm line of a molybdenum X-ray source?

(c) Which X-ray source gives you the better spacial resolution between the diffraction spots?

31-41. In this problem, we will derive the structure factor for a sodium chloride-type unit cell. First, show that the coordinates of the cations at the eight corners are $(0,0,0)$, $(1,0,0)$, $(0,1,0)$, $(0,0,1)$, $(1,1,0)$, $(1,0,1)$, $(0,1,1)$, and $(1,1,1)$ and those at the six faces are $(\frac{1}{2},\frac{1}{2},0)$, $(\frac{1}{2},0,\frac{1}{2})$, $(0,\frac{1}{2},\frac{1}{2})$, $(\frac{1}{2},\frac{1}{2},1)$, $(\frac{1}{2},1,\frac{1}{2})$, and $(1,\frac{1}{2},\frac{1}{2})$. Similarly, show that the coordinates of the anions along the 12 edges are $(\frac{1}{2},0,0)$, $(0,\frac{1}{2},0)$, $(0,0,\frac{1}{2})$, $(\frac{1}{2},1,0)$, $(1,\frac{1}{2},0)$, $(0,\frac{1}{2},1)$, $(\frac{1}{2},0,1)$, $(1,0,\frac{1}{2})$, $(0,1,\frac{1}{2})$, $(\frac{1}{2},1,1)$, $(1,\frac{1}{2},1)$, and $(1,1,\frac{1}{2})$ and those of the anion at the center of the unit cell are $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. Now show that

$$\begin{aligned}
F(hkl) &= \frac{f_+}{8}\left[1 + e^{2\pi ih} + e^{2\pi ik} + e^{2\pi il} + e^{2\pi i(h+k)} + e^{2\pi i(h+l)} + e^{2\pi i(k+l)} + e^{2\pi i(h+k+l)}\right] \\
&\quad + \frac{f_+}{2}\left[e^{\pi i(h+k)} + e^{\pi i(h+l)} + e^{\pi i(k+l)} + e^{\pi i(h+k+2l)} + e^{\pi i(h+2k+l)} + e^{\pi i(2h+k+l)}\right] \\
&\quad + \frac{f_-}{4}\left[e^{\pi ih} + e^{\pi ik} + e^{\pi il} + e^{\pi i(h+2k)} + e^{\pi i(2h+k)} + e^{\pi i(k+2l)}\right. \\
&\qquad \left. + e^{\pi i(h+2l)} + e^{\pi i(2h+l)} + e^{\pi i(2k+l)} + e^{\pi i(h+2k+2l)} + e^{\pi i(2h+k+2l)} + e^{\pi i(2h+2k+l)}\right] \\
&\quad + f_- e^{\pi i(h+k+l)} \\
&= f_+\left[1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l}\right] \\
&\quad + f_-\left[(-1)^h + (-1)^k + (-1)^l + (-1)^{h+k+l}\right]
\end{aligned}$$

Finally, show that if h,k,l are all even, we have the left case below; if h,k,l are all odd, we have the right case below; and otherwise, we have the center case below.

$$F(hkl) = 4(f_+ + f_-) \qquad F(hkl) = 0 \qquad F(hkl) = 4(f_+ - f_-)$$