1. **1D diffraction (similar to Kittel 2.4)** Consider a finite 1-dimensional chain of equally spaced atoms at positions $\vec{r}_m = ma\hat{x}$

   (a) Show that the magnitude square of the scattering amplitude

   $$|F|^2 = \frac{\sin^2 \frac{1}{2} N\vec{a} \cdot \Delta\vec{k}}{\sin^2 \frac{1}{2}\vec{a} \cdot \Delta\vec{k}}$$

   hint:

   $$\sum_{m=0}^{m=N-1} x^m = \frac{1 - x^N}{1 - x}$$

   (b) The diffraction condition occurs when $\vec{a} \cdot \Delta\vec{k} = 2\pi p$ (p integer). Show that the peak $|F|^2$ scales as N^2 and the width scales as $1/N$ (hint, consider what happens if $a\Delta k = 2\pi + \epsilon, \epsilon \ll 1$).

2. **Interplaner separation (based on Kittel 2.1)** Consider a plane hkl in a crystal lattice

   (a) Prove that the reciprocal lattice vector $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$ is perpendicular to this plane.

   (b) Prove that the distance between two adjacent parallel planes of the lattice is

   $$d(hkl) = \frac{2\pi}{|\vec{G}|}$$

   (c) Show that for a simple cubic lattice that

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

   (this is true for the fcc & bcc lattices as well, when we use the conventional unit cell).

3. **Structure Factor of bcc Lattice** The geometrical structure factor is given by

   $$S_{\vec{G}} = \sum_j f_j \mathrm{e}^{i\vec{G}\cdot\vec{r}}$$

   where $\vec{r_j}$ is the position of jth *atom* in the unit cell, and f_j is the atomic form factor of the jth *atom* (the scattering amplitude of a single atom, in units of single electron scattering).

   (a) Show that for the bcc structure with a single atom per primitive cell, that the structure factor reduces to

   $$\begin{aligned} S = 0 &\quad \text{when } h + k + l = \text{ an odd integer,} \\ S = 2f &\quad \text{when } h + k + l = \text{ an even integer} \end{aligned}$$

   when referred to in the conventional unit cell (i.e, two identical atoms, one at $r = 0\vec{a}_1 + 0\vec{a}_2 + 0\vec{a}_3$, and another at $r = (1/2)\vec{a}_1 + (1/2)\vec{a}_2 + (1/2)\vec{a}_3$)

   (b) What is the physical significance of the missing diffraction peaks when $h + k + l$ is an odd integer i.e, (100), (111), (300), etc.?

4. **Electron, neutron and x-ray (photon) diffraction** Diffraction from solids is not limited to x-ray radiation. Electron and neutrons may also be used, so long as their deBroglie wavelength (h/p) is short enough. Compare the energy and velocity of the longest wavelength radiation of diffraction for electrons, neutrons and photons from Na metal, given that it forms a bcc lattice with a cubic lattice constant of a =4.23Å.

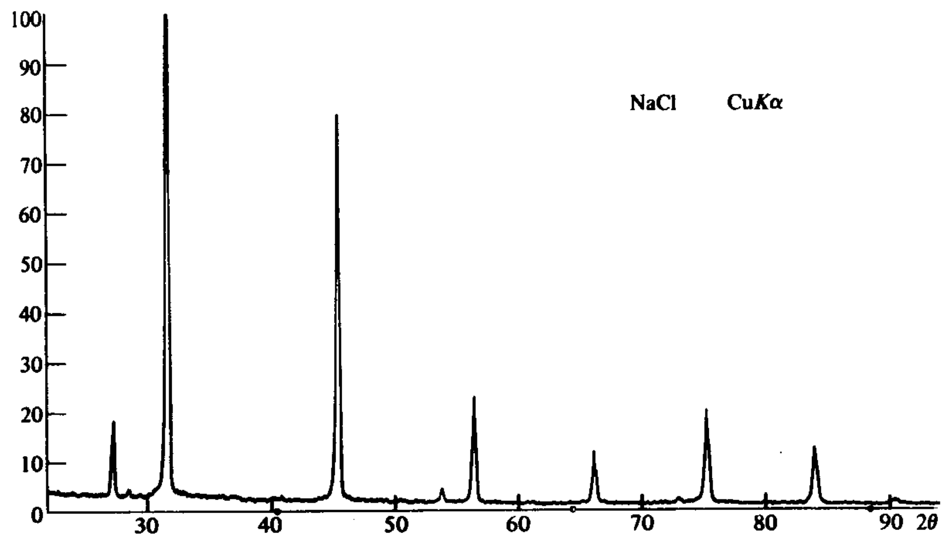

Figure 1: Powder diffraction pattern for NaCl, from Warren

5. **Powder Diffraction**

Figure 1 shows powder diffraction data for NaCl for $\lambda = 1.542$Å (Cu K_α radiation). In table 1, the angles, a geometrical polarization factor, and the area of each peak are tabulated.

Answer the following (filling in the table where appropriate):

(a) Identify the peaks in terms of their miller indices. What is the degeneracy, m, of the particular peak (i.e., how many possible permutations of hkl will give the same Bragg condition). Hint, this may take some trial and error. It may help to start with low orders of hkl and consider what the ratios would be for a cubic crystal.

(b) Verify that NaCl is face-centered cubic and determine the cubic lattice constant a (of the conventional cell)?

(c) The density of NaCl is 2.17g/cm^3, show that there are 4 Na and 4 Cl ions in the unit cell.

(d) Given that the structure is fcc, with 4 Na and 4 Cl ions, it turns out that the only two ways of placing the Na^+ and Cl^- ions in the unit cell correspond to the zinc-blende and the rock salt structure. By considering the strength of the diffraction peaks, verify that NaCl forms the rock-salt structure (aka NaCl).

(e) The area under the diffraction peak is expected to be proportional to the square of the structure factor, S^2, multiplied by the degeneracy, m, and a geometrical correction due to polarization effects, P (values of which are tabulated in table 1). Complicating matters is that the atomic form factors are functions of $\sin\theta/\lambda$ (see Kittel for explanation and my figure 2 for approximate values). When all of these factors are taken into account, how well do we reproduce the peaks in the data?

2θ	hkl	m	a	f_{Cl^-}	f_{Na^+}	$\|S\|^2$	P	$Pm\|S\|^2$	Area [arb]
27.3							33.5		116
31.7							24.0		1260
45.5							10.9		694
53.9							7.4		23
56.5							6.6		200
66.3							4.7		92
73.2							3.8		13
75.4							3.60		198
84.1							3.05		136
90.6							2.80		10

Table 1: NaCl powder diffraction data (from Warren)

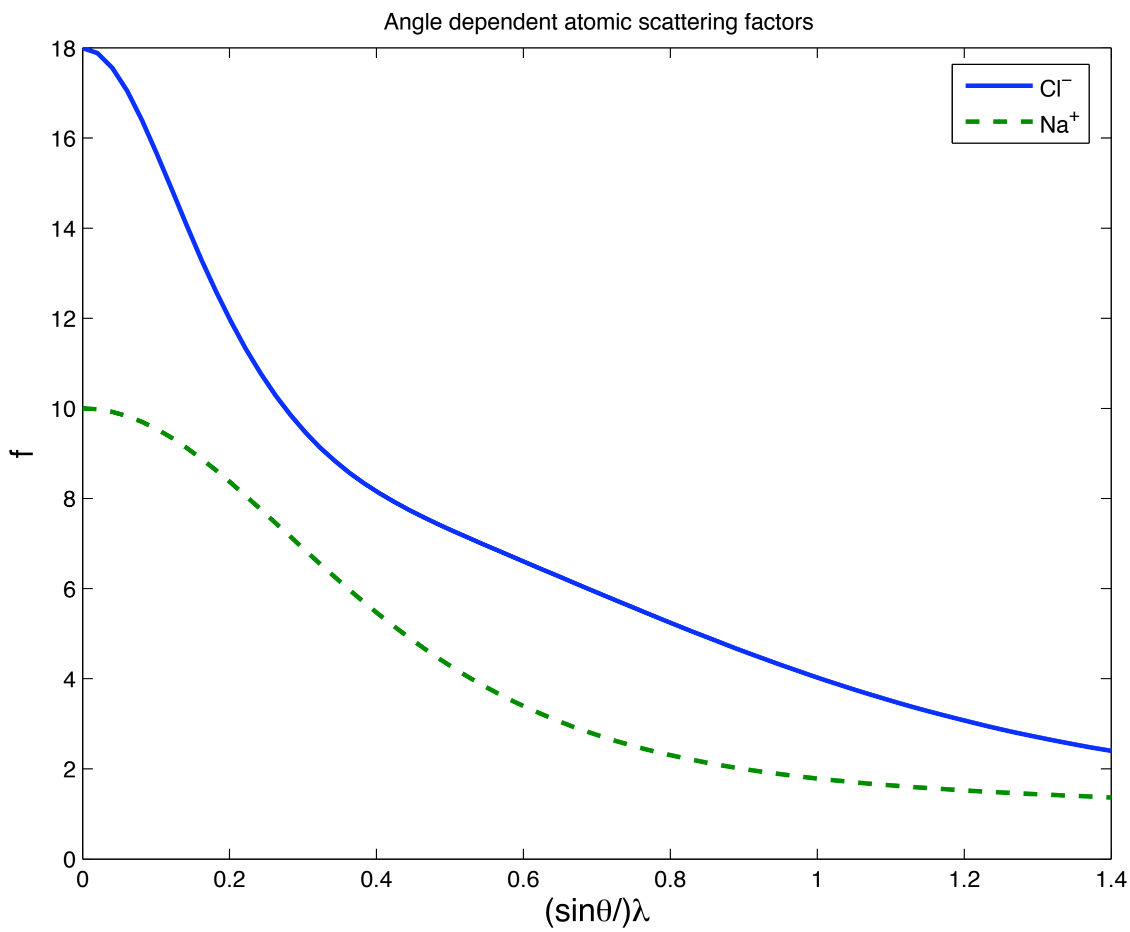

Figure 2: Atomic form factors for Na^+ and Cl^- ions as a function of angle

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