$$\rho = \frac{An}{N_{Av}\, a^3} \tag{3.16}$$

which can be solved easily for the lattice constant a:

$$a = \sqrt[3]{\frac{An}{\rho\, N_{Av}}} \tag{3.17}$$

Alternatively, if one assumes that the atomic data are known, then Eq. 3.16 can be used to calculate the theoretical mass density.

We will work out an example according to Eq. 3.17 using aluminum as the material. Al is an FCC metal, thus has $n = 4$, $A = 26.98$ g, and $\rho = 2.71$ g/cm^3. If we plug these values into Eq. 3.17 we get

$$a = \sqrt[3]{\frac{26.98 \times 4}{2.71 \times 6.02 \times 10^{23}}} = 4.05 \times 10^{-8}\text{cm} = 0.405 \text{ nm} \tag{3.18}$$

This is in fact equal to the literature value of the lattice constant for Al.

3.10.3 X-ray Diffraction of Ceramics

X-ray diffraction of ceramic materials can be dealt with similarly to metals. Now the complication is that X-rays scatter off of atomic planes containing different kinds of atoms, and these atoms scatter X-rays differently. Therefore, obtaining constructive interference is more complicated, and Bragg's Law, Eq. 3.13, will surely look different.

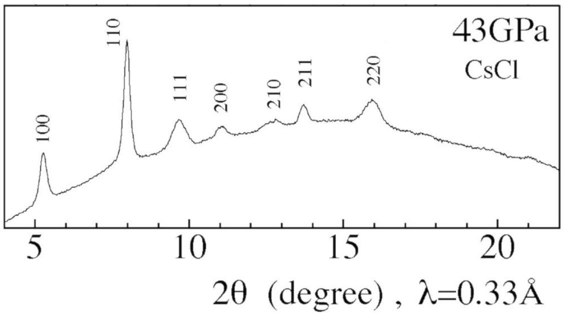

Figure 3.44: X-ray diffraction pattern of CsCl. Note that this is an SC pattern.

Instead of working this out in general, I will make a plausible qualitative argument using CsCl and KCl as examples. You recall that we described CsCl as simple cubic (SC) with a basis of two atoms, even though on casual inspection it looked like BCC (Fig. 3.19). So we would expect the diffraction pattern to be that of an SC structure. And indeed it is (Fig. 3.44).

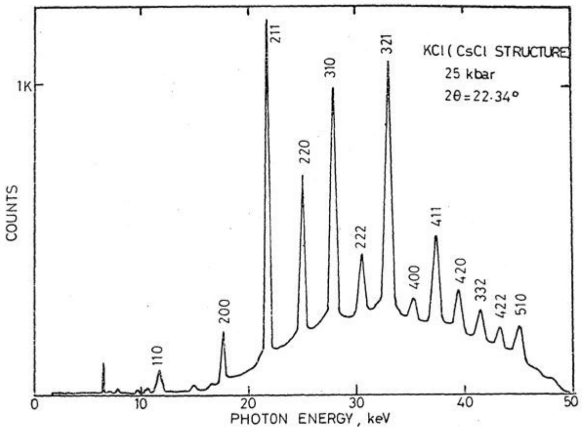

Figure 3.45: X-ray diffraction pattern of KCl. It looks like BCC: Only peaks with $h + k + l$ even are present.

But what about KCl? It also has the CsCl-type structure. In this case, it turns out that the K^+ and C^- ions are practically identical when it comes to scattering X-rays. This is, of course, because they have identical electron configurations. Therefore, the X-ray diffraction pattern of KCl does look like BCC, and indeed some of the SC peaks are missing!

Note that in Fig. 3.45 the diffracted beam intensity is plotted as a function of the X-ray photon energy, which means indirectly as a function of λ, at fixed θ. The X-ray source in this experiment was not a regular laboratory source, but a so-called synchrotron, which allows to vary λ continuously. If you want to check Bragg's Law, you can use the relationship

$$\lambda = \frac{hc}{E_{ph}} \tag{3.19}$$

where h is Planck's constant, c is the speed of light, and E_{ph} is the X-ray photon energy.

It is possible to work out X-ray diffraction from such structures as CsCl and KCl in general. The approach is first to consider the lattice, which determines the type of unit cell, and then to add the effect of having several, possibly different, atoms in a unit cell. The effect of these atoms is expressed in the form of what is called the structure factor. In this way, diffraction patterns of very complex structures have been analyzed and indexed.

3.10.4 Small Particles, Surfaces, and Amorphous Materials

We wrap up our discussion of materials structure by examining a few special topics we are prepared to appreciate now. All are areas of active research.

a) X-ray diffraction from small particles

When we discussed the principals of X-ray diffraction, one point we emphasized was that in order for interference of reflected beams to yield a sharp diffraction pattern, diffracted beams from a large number of planes (and atoms) had to interfere constructively. Conversely, this means that if the sample is small, the observed peaks may not be as sharp. Here is an example:

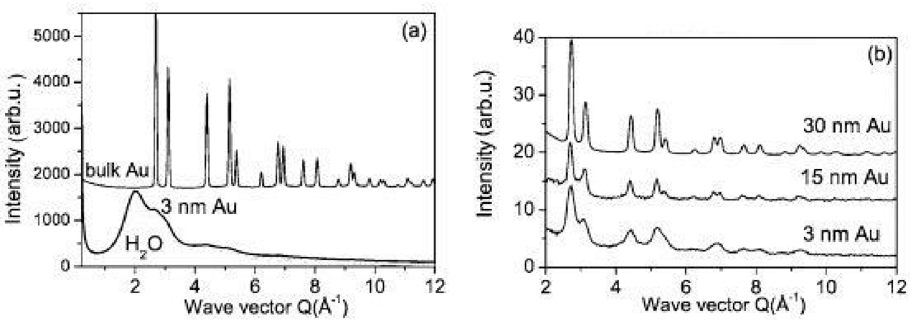

Figure 3.46: X-ray diffraction patterns of bulk Au, and small Au particles suspended in water.

Fig. 3.46a shows the diffraction patterns for bulk Au on top and for 3 nm Au particles suspended in water at the bottom. The diffraction peaks due to the Au particles are small modulations of the H_2O background curve. Fig. 3.46b shows diffraction patterns for particles with three different sizes, after the H_2O background has been subtracted. (The x-axis labeled Wave vector Q is essentially the same as $\sin \theta$). For particles, the small number of Au atoms scattering the X-rays not only causes a greatly reduced scattered X-ray signal, but also much wider diffraction peaks. (See also Fig. 3.43). With proper analysis, the width of the diffraction peaks can be used to determine the size of the particles.

Similar size effects can be observed in X-ray diffraction from very thin films of materials.

b) X-ray diffraction amorphous solids and liquids

After our focus on crystalline materials, you may be tempted to think that X-ray diffraction is useless for amorphous materials. That is not so: Amorphous materials do lack long-range order, but that does not mean that that there is no structure whatsoever over the short range, especially between a certain atom and its closest neighbors.