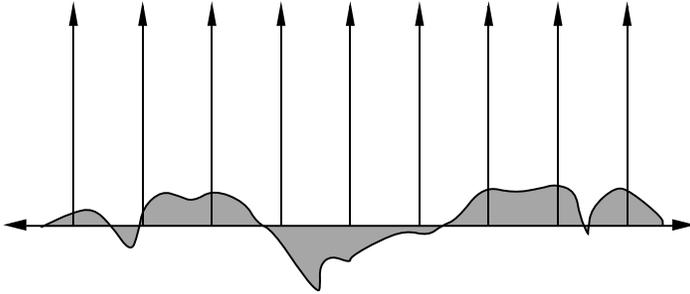# 9. Patterson Functions and Diffuse Scattering

9.1 The Patterson Function

9.1.1 Overview

Starting in Chapter 3, the kinematical theory of diffraction has been developed by calculating the diffracted wave from crystals with increasing amounts of disorder. The amplitude of the diffracted wave, ψ, is the sum of phase factors of wavelets emitted from individual atoms. We have evaluated these sums analytically (as a geometric series, for example), graphically (with a phase-amplitude diagram), and numerically. These calculations of $\psi(\boldsymbol{\Delta k})$ were performed for crystals having only small departures from ideality, such as crystals of small size, crystals with strain distributions, or isolated defects imaged with a TEM. In many respects these calculations were extensions of the calculation of wave interference from atoms in a perfect crystal. Recall that the phase information in $\psi(\boldsymbol{\Delta k})$ includes details of atom positions, which can be obtained by inverse Fourier transformation, $F^{-1}\psi$.

This chapter takes a different approach of calculating directly the diffracted intensity $I(\boldsymbol{\Delta k})$, rather than calculating it as $\psi^*\psi$. In this new approach, the real space information is obtained with the Fourier inversion $F^{-1}I$, rather than $F^{-1}\psi$, but this sacrifices some information about atom positions. Nevertheless, the intensity is the actual quantity measured in a diffraction experiment, so this new approach offers a more rigorous understanding of what

structural information is available from diffraction experiments. Furthermore, in cases of severely disordered materials, there may be no obvious way to obtain the atom positions needed for a calculation of $\psi(\boldsymbol{\Delta k})$. For problems involving severe structural disorder, another advantage of direct manipulations of $I(\boldsymbol{\Delta k})$ is that a convenient reference state will prove to be a homogeneous distribution of scatterers, or uncorrelated scatterers as in an ideal gas. A powerful tool for calculating diffraction intensities from such materials (and regular crystals too) is the "Patterson function," defined in Sect. 9.1.3 as an autocorrelation function of the scattering factor distribution.

Whereas the diffracted wave, $\psi(\boldsymbol{\Delta k})$, is the Fourier transform of the scattering factor distribution, the diffracted intensity, $I(\boldsymbol{\Delta k})$, is the Fourier transform of the Patterson function of the scattering factor distribution.

The Patterson function is a function in real space, with argument $\boldsymbol{r}$. The Patterson function is a convolution, so the reader should be familiar with convolutions and the convolution theorem (Sect. 8.1.3) before reading the present chapter. The work with convolutions in this chapter will help the reader through Chapters 10 and 11.

We begin by proving the emphasized statement above. The subsequent sections use the Patterson function to explain diffraction phenomena involving displacements of atoms off of periodic positions owing to temperature or atomic size. Diffuse scattering from chemical disorder is explained in detail. A radially-averaged Patterson function, the "radial distribution function," is used to describe amorphous materials.[1] The chapter ends by explaining small-angle scattering in terms of both the diffracted wave and the Patterson function.

The Patterson function lends itself readily to abstract manipulations, so many topics in this chapter are presented concisely. There is less emphasis on crystallography and more on formal manipulations. For this reason, we revert to the notation used in Chapters 3 and 4, where $k \equiv 2\pi/\lambda$ and $g \equiv 2\pi/d$. In this Chapter 9, phase factors are $\exp(\mathrm{i}\boldsymbol{\Delta k}\cdot\boldsymbol{r})$, rather than $\exp(\mathrm{i}2\pi\boldsymbol{\Delta k}\cdot\boldsymbol{r})$. For clarity, prefactors of $1/\sqrt{2\pi}$ are neglected in Fourier transformations when the absolute value of the diffraction intensity is unimportant.

9.1.2 Atom Centers at Points in Space

The most important results in this chapter are obtained by assuming the scatterers are points. At each point, $\boldsymbol{r}_j$, resides the scattering strength of one entire atom, $f_{\boldsymbol{r}_j}$ (or one unit cell). The atomic form factor, $f_{\mathrm{at}}(\boldsymbol{r})$, (or the structure factor of the unit cell) is included later by convolution, and does not change the essence of the results obtained with point atoms.

It proves convenient to consider a distribution of scatterers, $f(\boldsymbol{r})$, with a continuous variable, $\boldsymbol{r}$, rather than a sum over discrete points, $\{\boldsymbol{r}_j\}$. We

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[1] For powder diffraction patterns of crystals it is called the "pair distribution function," and was described qualitatively in Sect. 1.5.5.