# 1.1. Overview and principles of powder diffraction

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### 1.1.1. Information content of a powder pattern

The structures of real materials comprise not only the crystal structure – the time- and space-averaged periodic configuration of atoms on an idealized periodic lattice – but also the microstructure, which is caused by imperfections, dislocations and all kinds of disorder. The microstructure is often responsible for interesting properties of the material. A powder diffraction pattern contains a wealth of information about this microstructure in addition to the average crystal structure, as shown schematically in Fig. 1.1.1.

At each stage of a powder diffraction study, great effort and ingenuity are needed to find the optimal experimental conditions and to understand and analyse the resulting line shapes and signals. As experimental equipment, theoretical understanding and computational tools have improved, it has become possible to tap into the rich information content of the line peak shapes and diffuse background of a typical powder diffraction pattern, yielding unprecedented information about real materials for materials scientists, chemists, physicists, earth scientists and engineers. For example, in the modern practice of whole-pattern modelling, the line profile is calculated from first principles, taking into account all aspects of the state of the sample, such as particle-size distributions, inhomogeneous strains and texture, as well as the experimental setup and aberrations. There is a useful feedback effect in that better profile descriptions result in more accurate determinations of the intensities of the Bragg peaks, which is important to extract accurate structural information (Bragg peaks are introduced in detail in the next section). Similarly, great progress has been made in the extraction of information from the diffuse signal that used to be called the 'background'. Rather than fitting the background using arbitrary fitting parameters, as is done in a traditional Rietveld refinement, careful corrections can be made for experimental effects such as Compton scattering, fluorescence, multiple scattering and scattering from sample environments. The resulting 'background' beneath and between the Bragg peaks of the corrected data is information-rich diffuse scattering from the sample, which contains information about the local structure and how it deviates from the average crystal structure in the form of defects and correlated lattice dynamics (phonons). Total-scattering methods that include both the Bragg and diffuse scattering are only now being fully appreciated, with quantitative analyses being carried out in real space using the atomic pair distribution function (PDF) method, and in reciprocal space with Monte Carlo simulated-annealing-type modelling based on the Debye equation.

In this introductory chapter, the basic physics behind the observation of a powder diffraction pattern is described. In accordance with the scheme in Fig. 1.1.1, the information in a powder diffraction pattern can be described by the Bragg-peak positions, the peak profile, the Bragg-peak intensities and the non-Bragg-scattering contributions to the background. After describing the fundamentals of scattering by a crystalline powder, the chapter is organized such that each of the paths illustrated in Fig. 1.1.1 is followed and described in an introductory way. Detailed descriptions of the state of the art in the kinds of studies covered in Fig. 1.1.1 can be found in following chapters, but here we discuss each aspect of powder diffraction in turn, giving a high-level overview of what information is available from powder diffraction as well as explaining the fundamental origin of the features containing that information. We do not attempt to review applications of the different kinds of studies, leaving that to the following chapters.

In this chapter we have drawn heavily on information within three textbooks (Dinnebier & Billinge, 2008; Mittemeijer & Welzel, 2012; Egami & Billinge, 2013) and references therein.

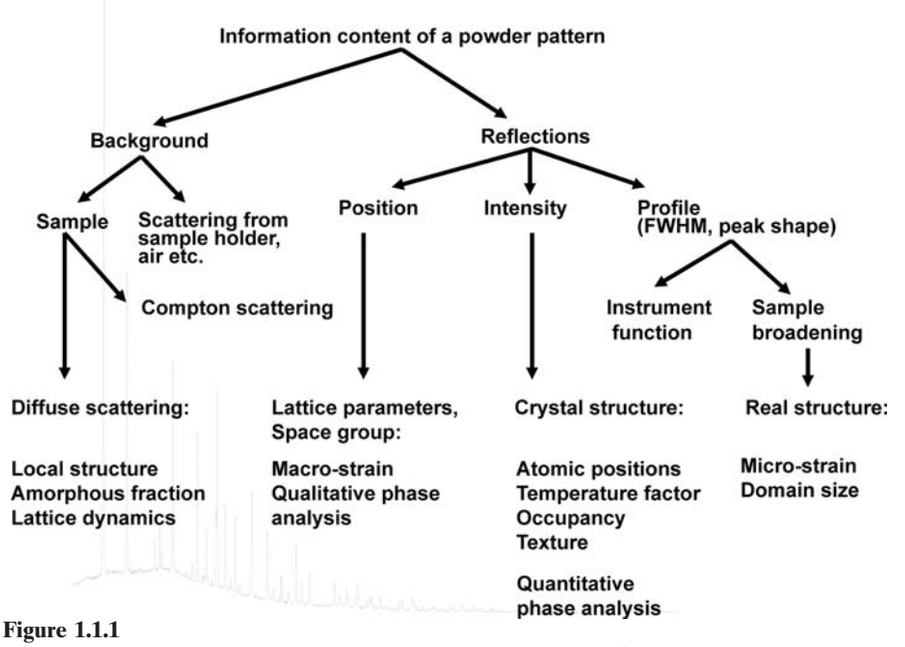


**Figure 1.1.1**
Schematic picture of the information content of a powder pattern. [Reproduced from Dinnebier & Billinge (2008) with permission from the Royal Society of Chemistry.]

### 1.1.2. The peak position

1.1.2.1. *The Bragg equation derived*

The easiest way to understand the structural information contained in powder diffraction, and historically one of the first ways in which diffraction was described, is *via* the well known Bragg equation (Bragg, 1913), which describes the principle of X-ray diffraction in terms of the reflection of X-rays by sets of lattice planes.

To understand the concept of a lattice plane, first imagine a three-dimensional periodic lattice of points, for example the corners of an array of cubes stacked in three dimensions. We can imagine a particular plane through the lattice by placing each layer of the stack of cubes on a tray: the tray then defines a lattice plane. Now imagine making the tray thinner and thinner until it



references