F.H. Chung & D.K. Smith, “Industrial Applications of X-Ray Diffraction”, Dekker, (2000), p21

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Industrial Applications of X-Ray Diffraction

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may be used: individual peak information, the complete set of d and I information, and as the whole trace. Individual peak information and the d–I set may be obtained from the trace by utilizing various peak-finding algorithms or by peak profile fitting using programs such as PRO-FIT (Toraya, 1986, 1993) and SHADOW (Howard and Preston, 1989). The full pattern may be analyzed for only the peak positions by programs such as WPPF, which fits the unit cell parameters for one or more phases to the trace. Programs such as that of LeBail, Duroy, and Fourquet (1988) may accomplish the extraction of the intensities for structure analysis. The full structure refinement may be carried out by many Rietveld programs (Young, 1993). It is also possible to graphically decompose patterns by superposing a reference pattern from a full-pattern database without processing the raw data in any way (Smith, Hoyle, and Johnson 1993).

It should be mentioned that there are two ways to extract information from a diffraction peak: decomposition and deconvolution. These terms are commonly misused, especially deconvolution. Decomposition is the separation of overlapped peaks by using a selected analytical profile and optimizing the fit of the cluster by adjusting the profile parameters. Deconvolution is the extraction of the sample contribution in a profile from the source and instrument contribution by elaborate mathematical methods that may involve some approximations. The profile-fitting procedures used for extracting position and intensity information involve decomposition. Separation of size and strain information by procedures such as the Warren–Averbach method involves deconvolution.

5. ANALYTICAL METHODS

Powder diffraction techniques may be classified into those that yield a qualitative answer and those that yield a quantitative answer. Qualitative answers include confirmation or identification of the phases present in a specimen and crude estimates of how much is present. Quantitative analysis provides numbers with estimated accuracy for crystallographic parameters including lattice dimensions, phase abundances, crystal structure coordinates, and other physical property data.

The data in the PDF are most commonly used for phase identification. It must be remembered, when using the PDF, that all the d–I tables are based on peak information. That is, the d's and I's are reported for the peak positions from the experimental trace, and the peaks in a cluster are not decomposed into individual components. When making comparisons of diffraction data with the PDF, one must use peak heights versus peak heights not peak areas versus peak heights (i.e., apples versus apples, not apples versus oranges).

5.1. Qualitative Phase Analysis

The identification of phases based on their powder diffraction pattern dates back primarily to Hanawalt and Rinn (1936) and became a common procedure when the Powder Diffraction File was published and contained sufficient data sets to yield matches. As the coverage of the PDF improves, phase identification also improves. It is impossible to locate a match for an experimental data set if the data for the phase in question are not included in the reference file.

Where the user only wants to confirm the presence of a phase in a sample, it is a simple matter to locate an appropriate reference powder diffraction pattern and collect the experimental data for comparison. The problem arises when the user has little or no information from which to start. Fortunately, the powder diffraction pattern can be a sufficient

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