Rietveld Analysis and Data for the Powder Diffraction File

Modern powder diffraction has seen increased application of the Rietveld method for the study of crystalline materials. This method is the best technique to extract the most information about the material from the powder diffraction data. The results provide structure, crystallinity, and physical property data on the phases under study with a significance considerably better than can be achieved by any previous analysis technique. There is, however, a major problem incorporating the reported results from Rietveld studies into the Powder Diffraction File where the primary application is for the identification of crystalline phases.

In Rietveld analysis, the data are the raw, unmodified digitized intensities in the diffraction pattern; in the PDF, the data are the extracted *d* spacings from the peak positions and the intensities which correspond to the peak heights of the resolved peaks. None of the currently available Rietveld programs is equipped with routines to extract the *d-I* information. Consequently, manuscripts based on Rietveld studies rarely report results that are truly analogous to the PDF *d-I* tables. This situation produces an enigma for the editors of the PDF and *Powder Diffraction*.

Rietveld manuscripts sometimes report a list of *d* spacings and intensities; however, the *d*'s are calculated from the refined unit cell and the intensities are either calculated or from decomposed profiles for individual peaks. Considerable experience in phase identification by users of the PDF reveals much difficulty using ideal *d* values and integrated intensities in the procedures based on peak data. In time, new procedures based on full-pattern matching will alleviate this difficulty, but those procedures are yet to be perfected. In the meantime, there is need to bridge this gap by some means so as not to lose the quality of Rietveld data and its value to the enhancement of the Powder Diffraction File database of diffraction data.

The International Centre for Diffraction Data has initiated an "R" quality category in the PDF for Rietveld data that is reported as calculated *d*'s and/or *I*'s. These data will be used if no peak data are presented. There are two alternatives available to authors to convert the Rietveld data to PDF type *d*'s and *I*'s. The first is to use "peak-finding" routines to reduce the digitized raw diffraction trace to the peak information. Such routines usually exist in the APD software and have been used to find the peak positions for finding the unit cell. Alternatively, there are several independent programs available in the public and commercial domain. The second approach is to use a program to generate the diffraction trace from the refined crystal structure parameters, and then generate a peak *d-I* list by an appropriate algorithm. Programs are also available in the public and commercial domains which follow this approach. Unfortunately, no such routine is presently incorporated into any Rietveld program to supply this type of output from the calculated data trace produced in the refinement procedure. It is left to the discretion of the authors to make the extra effort to do this separate step.

The problem at the moment is to convince authors that there is sufficient justification to extract peak *d-I* information during their Rietveld studies and to convince program suppliers that the appropriate routines are important components of the whole program package. The difficulty is at least in part due to the different goals of those researchers who use the Rietveld approach for analyzing the structural state of crystalline materials and the service diffractionist who needs to identify the phases in the materials supplied to the laboratory. An individual skilled at interpreting the parameters produced by a Rietveld study will usually be able to also apply the derived phase information to the problem of phase identification. Unfortunately, the reverse is less true because many service personnel are not sophisticated crystallographers.

Powder Diffraction will continue to consider manuscripts based on Rietveld studies and publish those papers which contain the *d-I* data in one of the above-mentioned forms. This editorial is a plea to authors to take the data processing as far as possible in their laboratory to provide the most useful form of *d-I* data obtainable.

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