Total Pattern Analysis Using PDF-4 Relational Databases: Instrumental Resolution, the Smith-Snyder Figure of Merit (SSFOM), and Total Pattern Analysis (TPA)

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The fundamental underpinnings for qualitative and quantitative phase analysis have rested with the description of diffraction results in terms of a concise peak-list, i.e., d-spacing/peak intensity (D-I) pairs. These are taken from the experimental data, usually after background subtraction and alpha-2 stripping. But the distillation of D-I pairs from experimental patterns is affected for example by instrumental resolution. The advent of new improved diffractometer designs (with considerable flexibility in choice of beam optics, insertion devices, sample geometry and detectors) and the advent of synchrotron instruments lead to a fairly wide range of instrumental resolutions. These developments will affect the reduction of experimental powder patterns to D-I pairs, and could affect D-I pair comparisons between experiment and the PDF. Moreover, information details concerning background variations, amorphous components in the scattering pattern, and peak-width information have been purposefully suppressed from consideration (e.g. stress/strain).

In this paper, we will follow these historical developments and show qualitatively how Bragg peak resolution affects the quality of pattern matching using Smith-Snyder FOM criteria [1]:

$$F_N = \frac{1}{|\Delta 2q|}\frac{N}{N_{poss}},$$

where N is the number of observed Bragg reflections, $|\Delta 2q|$ is the average $\Delta 2q$ error, and N_{poss} is the number of possible reflections. Specifically, we will use calculated patterns obtained from the ICDD PDF-4 databases and show how crystal symmetry and peak breadth affect the FOM. Residuals derived from unit cell least-squares analyses also correlate with these observations.

In contrast, we will examine methods for Total Pattern Analyses as implemented in DDView+, the front-end software in the PDF-4 relational databases [2-3]. We will explore how TPA helps us to recover search-indexing details that have been overlooked or lost using data reduction methods. Along the way, we will review several current developments in total pattern matching techniques.

[1] Smith, G. S. and Snyder, R. L., J. Appl. Cryst. 12, 60-65 (1979).
[2] J. Faber, C. A. Weth and J. Bridge, J. Powder Diffraction **19**, 26-30 (2004).
[3] T. G. Fawcett, S. N. Kabbekodu, J. Faber, F. Needham and F. McClune, J. Powder Diffraction **19**, 20-25 (2004).