FULL PATTERN COMPARISON OF EXPERIMENTAL AND CALCULATED POWDER PATTERNS USING INTEGRAL INDEX METHODS IN PDF-4+

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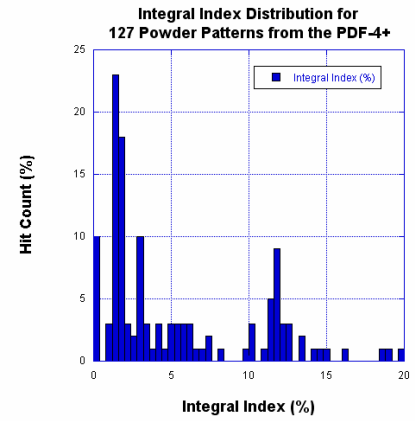
The fundamental underpinnings for qualitative and quantitative phase analysis have rested with the description of diffraction results in terms of a concise peak-list, i.e., d-spacing/peak intensity pairs. However, this reduced data (d,I pairs) does not conserve the full pattern information content (amorphous scattering, stress/strain and particle size effects). Recently, we have used on-the-fly technology to calculate fully digitized diffraction patterns for all entries in the PDF-4 [1]. Analytical profile models are used to take into account the instrumental resolution function and sample-dependent broadening. A recent addition to the peak shape function is to account for scattering from nano-phase materials [2]. DDView+ 2007, the front-end software for the PDF-4, provides 47 search functions so that the ~250,000 entries can be reduced to a manageable number of candidate patterns of interest. The task at hand is to facilitate comparison between an experimental pattern and a set of candidate, digitized patterns available in the PDF-4+ using DDView+.

Walter, Hofmann and Kuleshova [3] have discussed a new similarity index for crystal structure determination from X-ray powder patterns. We have applied this formalism to powder pattern matching, using DDView+. In this formalism, a perfect total pattern match gives a similarity index, SI=0%; a complete mismatch has SI=100%. Sample results are illustrated in the figure for SiC. The reference pattern exhibits a cubic structure. The 10 lowest Integral Index values are for patterns of cubic phase SiC. In this paper, we will describe the algorithm and it's application of search/match techniques applied to fully digitized powder patterns.



[1] J. Faber and T. Fawcett, Acta Cryst. **B58**, 325-332 (2002); J. Faber, Crystallography Reviews **10**, 97-107 (2004).
[2] P. Scardi, M. Leoni, and J. Faber, Powder Diffraction **21,** 270-277 (2006).
[3] D. Walter, M. Hofmann, and L. Kuleshova, J. Appl. Cryst. **38**, 861-866 (2005).