Total Pattern Analyses for Non-Crystalline Materials

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A wide range of programs and application tools have been developed for total pattern analysis. The total pattern analysis of crystalline materials is well developed, and the ability to identify materials and extract stress, strain and crystallite size as well as texture for each phase is a capability available in many commercial software programs. In addition, there are suites of programs that can solve structures from powder diffraction data and/or refine the structures for quantitative phase analysis.

For many classes of materials, particularly pharmaceuticals and minerals, there is an additional need to characterize non crystalline or poorly crystalline materials due to their common occurrence in routine samples. The International Centre for Diffraction Data, over a period of several years, has developed a system for analyzing whole patterns containing non-crystalline materials. The system includes several components; 1) the systematic addition of experimental pattern references for non-crystalline API's, clay minerals, polymers and excipients, 2) the development of application software that can correct for common instrumentation and specimen effects 3) a suite of graphics programs to scale, sum and display various combinations of reference and experimental data. These references and application programs are all embodied in the ICDD PDF-4 databases. Reference pattern simulations include adjustments for crystallite size and orientation. In this presentation we will describe the development tools and demonstrate their application for characterization of complex mineral and pharmaceutical specimens.