

SOFTWARE AND INSTRUMENTATION FOR RIETVELD ANALYSIS: WHAT'S NEW AND SOME PROGNOSTICATION

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In the past few decades, Rietveld analysis has moved from a niche technique used by a small number of crystallographers for structure determination ("desperate scientists do desperate things", J. Kaduk, unpublished communication) to a widely-used tool for a variety of other analyses: phase quantitation, stress and strain determination, crystallite size characterization and much more. Rietveld work demands high quality data, since resolution, sensitivity and data range all contribute to the quality of the results. Even with the best possible data, powder diffraction may not provide enough information to define all of a problem's free parameters, so adept use of constraints and restraints is often needed -- this requires versatile software.

The Rietveld technique was invented in Europe and many of the best facilities for powder diffraction are located there as well. However, for the first time in recent history, the United States can also offer new state-of-the-art user synchrotron and neutron facilities dedicated for powder diffraction. This talk will introduce them and I will offer some comments on where we will likely see progress. While lab instrumentation has also advanced significantly as well, this is better learned about in the exhibit hall.

The GSAS crystallographic analysis package, along with my personal contribution EXPGUI, has proven to be one of the most versatile and easiest to learn Rietveld packages and can be used with all types of powder and single-crystal diffraction data. There are a number of recent additions to EXPGUI worth hearing about.

The future will bring a versatile new package, GSAS-II, that will encompass powder diffraction data reduction as well as providing indexing tools and structure solution tools in addition to structure refinement. Progress and plans for GSAS-II will also be presented.