

Poster Presentation

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Processing Twinned-Modulated and Composite Structures from CCD / CMOS Images

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The Bruker APEX2 [1] software suite includes a full set of crystallographic programs for the solution and refinement of routine crystal structures. In addition to the standard tools required for routine problems, a number of advanced tools are also provided for analysis of non-merohedral twins and modulated structures. These tools include the CELL_NOW [2], SADABS [2] and TWINABS [2] programs and a Reciprocal Lattice Viewer with a q-vector analysis option. The Bruker SAINT [2] program is routinely used for the integration of image data collected with Bruker CCD (APEX II) or CMOS (PHOTON 100) two-dimensional detectors as part of the APEX2 software suite. SAINT has many advanced features for the processing of non-routine datasets. For example, a variety of new options have been implemented to facilitate the simultaneous integration of multiple domains for twinned and composite structures. Higher dimensional crystallography may be used to integrate modulated structures with up to three q-vectors. The output data for modulated structures may be output in either HKL5 or HKLF6 format suitable for input into the JANA2006[3] program. We will present results for one twinned-modulated structure and one composite structure to illustrate the use of the respective advanced options in SAINT to integrate images and JANA2006 to refine the structures.

[1] APEX2 (2014), Bruker AXS Inc., Madison, Wisconsin, USA, [2] SAINT (2014), CELL_NOW (2013), SADABS (2013), and TWINABS (2012), Bruker AXS Inc., Madison, Wisconsin, USA, [3] JANA2006 (2014), Vaclav Petricek, Michal Dusek and Lukas Palatinus, Institut of Physics, Academy of Science, Praha, Czech Republic

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