SXD2001 - a Program for Treating Data from TOF Neutron Single-crystal Diffraction

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In May 2001, the upgrade of the detector array of the time-offlight Laue single-crystal diffractometer SXD at ISIS has been completed and the detectors cover a solid-angle of 2π steradians. To meet the needs for data processing a new IDL based program, SXD2001, has been developed.

SXD2001 incorporates various visualisations for raw data and provides a complete route from indexing to intensity extraction and export to structure refinement programs in user friendly graphical interface. File formats suitable for GSAS, FULLPROF, SHELX and JANA2000 are supported. In addition, reciprocal space volumes can be displayed and arbitrarily sliced. Planar cuts or complete volumes can be exported.

Recent examples of science will be shown, including magnetic structure solution and diffuse scattering analysis.

Keywords: data analysis, Laue diffraction, neutron diffraction