MS30-01 **Discover the Cosmos of Reciprocal Space – Twins as a Routine Case?** Ina Dix, *Novartis Institutes for Biomedical Research, 4002 Basel, Switzerland,*
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The term 'twinned crystal' is frequently used if irregularities (e.g. split reflections) in the diffraction pattern are observed. Twins can be classified as merohedral, pseudo-merohedral, reticular merohedral and non-merohedral. As a consequence of the presence of several individual crystals of the same species joined together in some definite mutual orientation (Giacovazzo), problems occur during different steps of structure determination depending on the type of twinning: indexing, space group determination, structure solution and refinement. This presentation will focus on the class of non-merohedral twins.

The introduction of area detector technology in single crystals X-ray structure determination in the 1990s promoted the general awareness of non-merohedral twinning. Modern software development has also facilitated the handling of twinned data. The satisfactory description of a twinned crystal involves the determination of (i) the twin law, which defines the mutual orientation of the different components, and (ii) the fractional contribution of each component. The various steps of the analysis are supported by appropriate software components: from visualisation of diffraction data in RLATT [1] via automated indexing and determination of the twin law with CELL_NOW [2]; parallel data reduction of more than one species with SAINT [3] (dividing reflections into three groups: exact overlap, no overlap and partial overlap, with approximate determination of the fractional contributions); absorption correction, scaling and merging with TWINABS [4]; and structure refinement with an HKLF5 format file in SHELXL [5] if required. All these programs are part of the Bruker APEX 2 Suite [6].

Some examples of twinned structures will be presented, including advice for recognition of twinning and optimisation of data collection. We wish to demonstrate that the earlier negative attitude to twins can frequently be transformed into a positive outcome, whereby a publishable structure is obtained despite twinning and in addition two independent data sets are measured investing time for only one data set.

[1] Bruker (2000). RLATT, Bruker AXS Inc., Madison, Wisconsin, USA.
[2] Sheldrick, G. M. (2008). CELL_NOW, University of Göttingen, Germany.
[3] Bruker (2006). SAINT, Bruker AXS Inc., Madison, Wisconsin, USA.
[4] Sheldrick, G. M. (2009). TWINABS, University of Göttingen, Germany.
[5] Sheldrick, G. M. (2003). SHELXL V6.14, University of Göttingen, Germany.
[6] Bruker (2011). APEX2 V2011.4-1, Bruker AXS Inc., Madison, Wisconsin, USA.

Keywords: twinning; data treatment; SHELX

MS30-02 **Twin refinement with Jana2006: from polytypism to modulated phases.** Berthold Stöger[a] [a] *Vienna University of Technology, Institute for Chemical Technologies and Analytics, Austria*
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Twinning is the association of equivalent crystal individuals of different orientations related by a "well defined" orientation relation[1]. The occurrence of twinning has crystallo-chemical reasons and therefore analysis of twinning is an essential part of the structural characterization. Twinning is closely related to symmetry: On one hand, diffraction patterns of twins can feature higher symmetry than the pattern of the individuals. On the other hand, twins are most likely to appear in cases where the crystal lattice or parts of the structure feature higher symmetry than the overall structure. Therefore, twinning is commonly observed in merohedral crystal classes, super structures, incommensurates and polytypic structures. The advent of two dimensional detectors spurred new software developments and great progress has been made in the last decade concerning the refinement of crystal structures from twins. Yet, special care has to be taken during recognition, data reduction, structure solution, refinement and post processing of twins. The treatment of twins with the JANA2006 software package[2] will be exemplified with a few members of the thortveitite family, which features a rich crystal-chemistry with commensurately modulated, incommensurate and polytypic phases.

[1] Hahn, Th. & Klapper, H. (2006). *International Tables for Crystallography Vol. D*, Ch. 3. 3.

Keywords: twinning; incommensurate structures; polytypism