Oral Contributions

[MS11] Twinning: problems and advantages

Co-Chairs: Loes Kroon-Batenburg (NL), Pietro Roversi (UK)

[MS11-01] Layered molecular structures: The crystal chemistry of the twin interface.

Berthold Stöger,[a] Daniel Lumpi,[b] Paul Kautny[b]

[a]*Institute of Chemical Technologies and Analytics, Vienna University of Technology, Getreidemarkt 9/164-SC, Vienna, Austria.* [b]*Institute of Applied Synthetical Chemistry, Vienna University of Technology, Getreidemarkt 9/163-OC, Vienna, Austria.*
E-Mail: bstoeger@mail.tuwien.ac.at

Twinning is the association of equivalent domains related by a crystallographic twin law.[1] By definition, the specific orientation relation of the domains appears frequently, *i.e.* it is a structural feature. Twinning is a multifarious phenomenon, appearing in all classes of crystalline materials, ranging from minerals to bio-macromolecules. Twinning represents a possible first step from a perfectly ordered structure to disordered systems. Nevertheless, since the diffraction patterns of twins are discrete, the routine methods for structure solution and refinement can be applied with minor modifications. Thus, the analysis of twinning provides an insight into non-periodic systems.

The interesting part of a twin is the twin interface. It features a different, but energetically similar, arrangement of atoms compared to the twin individuals. It can be chemically identical or different from the individuals and likewise be geometrically equivalent or non-equivalent to the bulk of the individuals.

A phenomenon closely related to twinning is polytypism, *i.e.* the ability of a structure to crystallize with the same layers arranged in different ways. Polytypes are prone to crystallize as twins, whereby a fragment of a different polytype is located at the twin interface. We synthesized several π-spacer extended ene-yne compounds capped with silyl groups. By choosing para-substituted aryl spacers, we obtained a series of rigid linear molecules. All of them crystallized in distinct molecular layers delimited by the silyl groups. They feature a rich crystal chemistry ranging from polymorphism over incommensurate modulation to polytypism and twinning. The crystallo-chemical reasons of the twinning will be analyzed.

[1] Th. Hahn and H. Klapper, *International Tables for Crystallography* (2006). Vol. D, *Phsical Properties of Crystals,* Chapter 3.3

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