**o.m4.01** Symmetry relations between twin domains and experimental methods of their determination. H. Klapper<sup>1</sup>, Ch. Scherf<sup>2</sup>, Th. Hahn<sup>2</sup>, G. Heger<sup>2</sup>, N.R. Ivanov<sup>3</sup>. <sup>1</sup>Mineralog.-Petrolog. Institut, University of Bonn, D-53115 Bonn, Germany; <sup>2</sup>Institut fuer Kristallographie, RWTH Aachen, D-52056 Aachen, Germany; <sup>3</sup>Shubnikov Institute of Crystallography, Russian Acad. of Sciences, 59 Leninskii Prospect, Moscow 117333, Russia.

Keywords: twinning, phase transition, X-ray topography.

The orientation states of twin components (domains) are connected by (>twin=) operations which are closely rela-ted to the lattice of the crystal (i.e. reflections across a lattice plane (hkl) or normal to a lattice row [uvw], etc.). For growth twins (and with restrictions for deformation twins) these `orientation relationsA can often be recog-nized by morphological features (e.g. re-entrant edges). In any case (growth, deformation, transformation twins), different orientation states can be distinguished by the study of certain anisotropic physical properties, including X-ray diffraction. In the rather simple case of twins with non-parallel lattices (non-merohedral twins, ferroelastic twins), different orientation states are easily detected by the different orientations of the index ellipsoids (different `optical extinctionA positions) and by the splitting of X-ray diffraction spots. More subtle is the distinction of domains in merohedral twins, where a splitting of optical extinction positions and X-ray diffraction spots does not occur. Here other effects on physical properties (reversal of electrical axes and of optical rotation, change of X-ray diffraction intensities) have to be analysed. This is illustrated for GaPO<sub>4</sub> (quartz-homeotypic berlinite structure, point group 32) which exhibits growth twins with the three different twin laws: Dauphin & law (2-fold twin axis parallel [001]), Brazil law (inversion twin) and combined or Leydolt law (twin mirror plane (0001), no reversal of electrical axes). They define four domain states characterized by the orientation of the electrical axes, optical rotation sense and orientation of trigonal etch pits on (0001). These four domain states and their symmetry relations (twin laws) can unambiguously be determined by analysing the optical rotation sense and the orientation of electrical axes or of the etch pits. Moreover, all domains can be imaged and their symmetry relations can be determined by X-ray diffraction topography using certain pairs of reflections related by the twin operation. This is easily achieved by white-radiation synchroton Laue topography, which allows the record of many topographs in different reflections within one shot. The analysis of the various growth and transformation twins of KLiSO4 and NH<sub>4</sub>LiSO<sub>4</sub> by conventional X-ray and synchroton Laue topography and by a novel technique of nematic liquidcrystal (NLC) surface decoration is demonstrated. An outstanding example is the twinning which results during the transition of KLiSO<sub>4</sub> from phase III (point group 6) into phase IV (point group 3n) with twin law "2-fold axis parallel [001]": the twin domains cannot be distinguished optically but are imaged and unambiguously characterized by X-ray diffraction topography.

o.m4.02 Anomalous structure states in real ferroic crystals. I. M. Shmytko, Institute of Solid state Physics, Chernogolovka, Moscow distr., 142432, RUSSIA e-mail: shim@issp.ac.ru Keywords: twinning.

The following anomalous structure states in ferroic crystals will be outlined:

**1**. - the structure of the twin boundaries in the form of transitional regions along which the structure parameters of one twin orientation continuously and smoothly are transformed into the crystallographic parameters of the other twin orientation<sup>1</sup>. The energetic aspects of the emergence of such transitional regions will be reviewed. The experimental observation of such intertwined regions (received with help of X-ray and electron micro diffraction methods) will be demonstrated on the examples of ferroelectric crystals BaTiO<sub>3</sub> and KH<sub>2</sub>PO<sub>4</sub> and HTS compounds ReBa<sub>2</sub>Cu<sub>3</sub> O<sub>x</sub>, where Re = Y and Gd. The quasi twins as a limit of intertwined boundary thickness compared with sizes of twins will be shown on the example of HoBa<sub>2</sub>Cu<sub>3</sub> O<sub>x</sub> crystal;

**2**. - the phase transition in such twin boundaries will be demonstrated on the example of  $CsDy(MoO_4)_2$  crystals;

**3**. - the observation additionally to famous twin structure in  $\text{ReBa}_2\text{Cu}_3 \text{ O}_x$  compounds of the not centrosymmetrical domains will be demonstrated with help of Borrmann effect and traditional structure analysis;

**4**. - the presence of interpenetrated twin systems will be demonstrated on the example of twin structure in LaGaO3 single crystals;

5. - defect density waves and specific manifestations of the memory effects like phase- and amplitude correlation of the "incommensurate domains " will be demonstrated on the example of incommensurately modulated phases in  $SC(NH_2)_2$  and TMA-ZnCl<sub>4</sub> crystals<sup>2</sup>;

**6**. - twinning and detwinning in politype crystals with help of partial dislocations will be demonstrated on the examples of ZnS and Si crystals.

<sup>[1]</sup> I.M.Shmyt'ko and V.Sh.Shekhtman "Twins, and Structure of Twin Boundaries", in Springer Series in Materials Science,, "The Real Structure of High-Tc Superconductors" Springer-Verlag Berlin Heidelberg (1993), Vol. 23, pp. 23-43.

<sup>[2]</sup> I.M.Shmyt'ko and B.Sh.Bagautdinov "Defect Density Waves and Specific Manifestations of the Memory Effect in the Crystals with Incommensurate Phases", Crystallography reports, (1998), Vol. 43, pp. 631-639.