

Phase boundaries and domain boundaries in crystals

H KLAPPER, TH HAHN[†] and H-D JENNISEN[†]

Mineralogisches Institut, University of Bonn, D-5300 Bonn, [†]Institut fuer Kristallographie der RWTH Aachen, D-5100 Aachen, Germany

Abstract. Domain boundaries, i.e. interfaces between different orientation variants of the same crystal species, and phase boundaries, i.e. interfaces between two different modifications of the same compound, exhibit rather similar features. This has been investigated by means of polarized light and X-ray topography for a series of structurally related sulphates which were grown as large single crystals from aqueous solution. The major results are as follows:

- (i) Domain interfaces frequently adopted only a few orientations which are low-energy boundaries of best structural fit. These preferred orientations may be parallel to low-indexed lattice planes or to non-crystallographic planes (*W* and *W'* walls according to the classification of Sapriel, *Phys. Rev. B*12, 1975, 5128). Illustrations of such (transition-induced) domain boundaries in KLiSO_4 , NH_4LiSO_4 , RbLiSO_4 , CsLiSO_4 , $(\text{NH}_4)_3\text{H}(\text{SO}_4)_2$ will be presented.
- (ii) For many first-order transitions the phase boundaries prefer planes of minimum strains, i.e. low energy, which again may be low-index lattice planes or non-crystallographic planes. These preferred orientations can be calculated from the strain tensor of the transition with the relative lattice-parameter changes as tensor components). If the transition isotherm deviates from the minimum strain orientation, characteristic zigzag boundaries with segments parallel to the (symmetrically equivalent) preferred planes may result. Zigzag phase boundaries have been observed in RbLiSO_4 and $\{\text{N}(\text{CH}_3)_4\}_2\text{ZnCl}_4$.
- (iii) The shape and the density of transition-induced domains is influenced by the orientation of the phase boundaries and its velocity of motion. For the 708 K transition of KLiSO_4 and the 413 K transition of $(\text{NH}_4)_3\text{H}(\text{SO}_4)_2$ (in both cases loss of the trigonal axis), among the minimum-strain domain boundaries those normal to the phase boundary are preferred. In $\{\text{N}(\text{CH}_3)_4\}_2\text{ZnCl}_4$, the domain density increases with the phase boundary velocity.