Microsymposium

MS17.O01

Twinning and Pseudosymmetry at High Pressures

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Twinning is a common known problem in the study of crystal structures from single-crystal data and often related to a high degree of pseudosymmetry of the structure with respect to a higher symmetrical parent one. With the rising popularity of in situ single-crystal diffraction studies under high pressure, the occurrence of twinned structures is more and more frequently reported. In this contribution, we review the available information on merohedral and pseudomerohedral twinning as well as pseudosymmetry under high pressures [1]. For twinning by merohedry type I (inversion twinning), a reliable characterization of the twin domains and volume fractions is difficult and largely depends on the experimental conditions, i.e., on the number of measured Friedel pairs and the chosen wavelength. For twinning by merohedry (type II) and for twinning by pseudomerohedry, twin volume fractions could be reliably determined from high-pressure data for several cases. In none of these, a significant influence of hydrostatic pressure on the volume fractions of the individuals was observed. Pressure-induced twinning has also been observed for compounds which undergo first-order phase transitions. It is remarkable that the twinning operation in such cases is related to the loss of rotational symmetry elements of the higher symmetrical polymorph, although the high- and low-pressure phases are not in the group-subgroup relationship. The analysis of pseudosymmetry of several compounds as a function of pressure suggests that this parameter can be used to predict the (in)stability of compounds. In particular, a decrease in pseudosymmetry seems to be strongly correlated with the occurrence of first-order phase transitions in which the crystals break or amorphize.

[1] *K. Friese, A. Grzechnik, Z. Kristallogr., 2014, in print, DOI: 10.1515/zkri-2013-1662*

Keywords: High pressure, Twinning, single crystal diffraction