

s5.m15.p4 **Lattice aspects of crystal twinning.** H. Grimmer, *Laboratory for Neutron Scattering, ETHZ and PSI, CH-5232 Villigen PSI, Switzerland. E-mail: hans.grimmer@psi.ch*

**Keywords: Twinning; Coincidence site lattices; Mallard's law**

Assume that the two individuals forming a twin are related by a mirror reflection parallel to a rational plane  $(hkl)$  or by a  $180^\circ$  rotation with axis parallel to a rational direction  $[uvw]$ . Mallard's "law" states that in both cases these elements can be complemented to a pair  $(hkl)$ ,  $[uvw]$  of rational elements, such that the angle between  $[uvw]$  and the normal to  $(hkl)$ , called the obliquity  $\delta$ , satisfies  $\delta \leq 6^\circ$  and that the twin index  $\Sigma$  is a positive integer not larger than 6 [1,2].

Discussing examples, especially of crystals with symmetries higher than orthorhombic, we shall show that this criterion is often satisfied for growth twins originating from a twinned nucleus. Growth twins formed by coalescence of two single crystals can better be described if stricter limits are imposed on  $d$  and less strict ones on  $\Sigma$ . If  $(hkl)$  is interpreted as the habit plane  $K_1$  of a mechanical twin and  $[uvw]$  as  $\eta_2$ , the observed values of the shear show that the restriction on  $d$  has to be relaxed at least for  $\Sigma = 1$  [3].

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- [3] H. Grimmer & K. Kunze, *Twinning by reticular pseudo-merohedry in trigonal, tetragonal and hexagonal crystals* (submitted to *Acta Cryst. A*).

s5.m15.p5 **The crystal structure and chemical composition of As-rich holtite.** S.S. Kazantsev<sup>a</sup>, D.Yu. Pushcharovsky<sup>b</sup>, M. Pasero<sup>c</sup>, S. Merlino<sup>c</sup>, N.V.Zubkova<sup>b</sup>, Yu.K.Kabalov<sup>b</sup>, A.V.Voloshin<sup>d</sup>, *Institute of Crystallography RAS, Russia, <sup>b</sup>Geology Department, Moscow State University, Russia, <sup>c</sup>Dip. de Scienze della Terra, Univ. di Pisa, Italia, <sup>d</sup>Institute of Geology, KD RAS, Russia. E-mail: kaiser@ints.ru*

**Keywords: Holtite; Frameworks; Crystal structure**

Holtite  $(\text{Ta,Al})\text{Al}_6(\text{BO}_3)(\text{Si,Sb,As})_3\text{O}_{12}(\text{O,OH})_b$  [1], discovered in 1971 in Western Australia, nowadays is present in pegmatites of two more locations. Two different specimen were found during the study of the chemical composition of As-rich holtite from Vorony Tundry (Kola peninsula), different in Sb content: low-Sb holtite I (earlier one) and hi-Sb holtite II (later one). The crystal structure of holtite I is refined (Ital Structures diffractometer, 939 independent reflections, anisotropic approximation,  $R=0.047$ ). The resulting formula  $(\text{Si}_{2.43}\text{Sb}_{0.36}\text{As}_{0.21})\text{BO}_3[(\text{Al}_{0.62}\text{Ta}_{0.26})\text{Al}_2(\text{Al}_{0.98})_2(\text{Al}_{0.94})_2\text{O}_{12}](\text{O,OH})_{b,65}$  is of good sequence with the microprobe analysis. The crystal structure of holtite and Al-Ta alternation in hexagonal tunnels is confirmed. This alternation is accompanied with the replacement of  $(\text{Si,As})\text{O}_4$  tetrahedra by the  $[\text{SbO}_3]$  pyramids. This replacement is of good sequence with the partially vacant O(2) and O(7) positions and high thermal parameters for these oxygen atoms. Positions are named after [3]. Attempts to find a single crystal of holtite II failed. To figure out its difference two X-ray patterns were obtained from the powders of holtite I and holtite II. Known crystal structure of holtite I was used in refinement of both patterns using Rietveld methods. For the holtite I pattern the resulting factors of instability are  $R_{\text{wp}} = 2.70\%$ ,  $R_F = 2.97\%$ ,  $S = 1.23$  and the single crystal model of the crystal structure is confirmed. However, the refinement of the powder pattern of holtite II was unstable. Authors can only state the structural difference of the two specimen. This work was supported by Russian Foundation for Basic Research (03-05-64054) and the "Russian Universities" program.

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