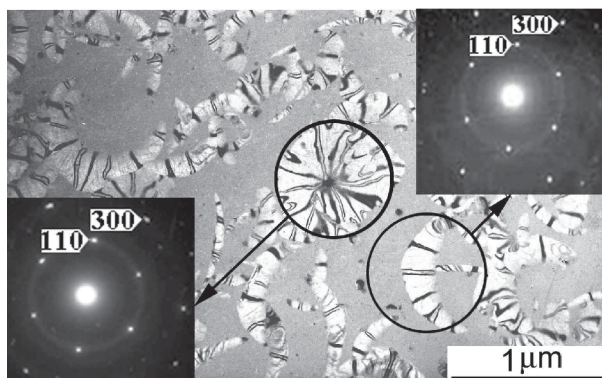


s4.m14.p1 **Orientational studies of Cr₂O₃ microcrystals growing in amorphous films by means of TEM bend contour technique.** V. Yu. Kolosov,^a C. L. Schwamm^a and A. G. Bagmut^b, ^aPhysics Dept., Ural State Economic University, Ekaterinburg, Russia, and ^bNational Technical University "KhPI", Kharkiv, Ukraine. E-mail: vladkol@usue.ru

Keywords: Electron microscopy and diffraction; Lattice orientation; Thin films

Bend contour technique [1] is very useful for transmission electron microscopy studies of lattice orientation, in particular for "transrotational" [2] crystals with internal lattice bending. The α -Cr₂O₃ crystals grown (400° C, 5 min.) in laser evaporated amorphous films are of 2 main morphology types:



round and crescent-like, Fig.1. [001] in the nucleus is, correspondingly normal and declined from the normal (through angle β) to the film plane. Contrary to selected area diffraction (giving the point patterns of the same lattice orientations) detailed analysis for "transrotational" crystals based on comparison of experimental micrographs and theoretical bend contour patterns (similar to stereographic projections of lattice planes) refines lattice orientations of crescent-like crystals ($\beta=12\div 26^\circ$). Furthermore, it makes possible to study the relationship between parameters of internal lattice bending and parameters of crystal morphology for the crystals studied. We suppose that it is the strong (about 90 degrees per micrometer of crystal length) internal lattice bending (around the axis lying in the film plane) revealed from the bend contour patterns, that determines most of the regularities observed.

- [1] V. Yu. Kolosov *Proc. XIII ICEM, Seattle*, San Francisco Press, v.1 (1990), p. 574.
- [2] V. Yu. Kolosov and A.R. Tholen, *Acta Mater.* **48** (2000), p. 1829.
- [3] This work is partially supported by INTAS (00-100), pending support from RFBR (04-02-96072/16656)

s5.m15.p1 **Schlegelite, the first naturally occurring bismuth-molybdate-arsenate.** Effenberger H.^a, Krause W.^b, Bernhardt H.-J.^c, ^aInstitut für Mineralogie und Kristallographie, Universität Wien, Althanstraße 14, A-1090 Vienna, Austria, ^bHenriette-Lott-Weg 8, D-50354 Hürth, Germany, ^cInstitut für Mineralogie, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum, Germany. E-mail: herta.silvia.effenberger@univie.ac.at

Keywords: Schlegelite; Crystal chemistry; Crystal structure

Schlegelite, ideally Bi₇O₄(MoO₄)₂(AsO₄)₃, is a new mineral from the dumps of the Pucher Richtschacht (near Schneeberg, Saxony, Germany). It forms yellow spherical aggregates up to 1 mm in diameter that are composed of small orthorhombic lath-like crystals elongated parallel to [100] and flatted on {010}, their length is less than 0.3 mm. Schlegelite is non-pleochroic, biaxial negative, $2V = 40(5)^\circ$, $n_x = 2.22$, $n_y = 2.255$ (calc.), and $n_z = 2.26$ (calculated from reflectance data), orientation $X = a$, $Y = b$, $Z = c$. The empirical formula is Bi_{6.78}Pb_{0.05}Ca_{0.02}O_{3.51}(MoO₄)_{1.90}(PO₄)_{0.16}(VO₄)_{0.05}(AsO₄)_{3.01}.

The space group is *Pnca*, $a = 5.299(1)$, $b = 16.133(4)$, $c = 23.948(5)$ Å, $V = 2047.2(7)$ Å³, $Z = 4$, $D_{\text{calc}} = 7.23$ g/cm³. The crystal structure investigation is based on 3021 unique / 2576 observed reflections measured with MoK α radiation in the 2θ range $< 60^\circ$, the crystal size was $8 \times 42 \times 130$ μm . The refinement converged at $wR2(F^2) = 0.130$ and $R1(F) = 0.058$. There are each four crystallographically independent Bi and X = Mo, As, P atoms. Parts of them (atoms Bi1, X1, X2, and X3) are located on two-fold axes; the atoms Bi2, Bi3, Bi4, X4, and all the O atoms are on general positions. Ten O atoms belong to the XO₄ groups; the two oxo-oxygen atoms are coordinated exclusively by Bi atoms. The Bi atoms exhibit a one-sided coordination to account for the space requirements of the lone-pair electrons. The ligands of the Bi1^[(2+2)+4] atom are in a bonding distance of ~ 2.24 Å, 2x, and 2.42 Å, 2x; the further ligands have Bi1-O > 2.65 Å. The other Bi atoms are [3+5] coordinated with the nearest ligands between 2.12 and 2.32 Å; the Bi-O distances in the second coordination sphere range from 2.51 to 3.12 Å. The shortly bound ligands are oxo-oxygen atoms. Only for the Bi1 atom the coordination is solely formed by O atoms belonging to the XO₄ tetrahedra.

The four XO₄ tetrahedra are distinct: the X1O₄ and X2O₄ tetrahedra are larger and stronger distorted as compared to the X3O₄ and X4O₄ tetrahedra going along with an occupation by solely Mo and predominantly As atoms, respectively. The average $\langle \text{Mo1} / \text{Mo2-O} \rangle$ bond lengths of $1.790 / 1.825$ Å compare well with the expectations for a pure MoO₄ tetrahedron. The X1 and X2 atoms show further interactions with each two additional ligands at 2.549 and 2.322 Å. The average $\langle \text{X3} / \text{X4-O} \rangle$ bond lengths are $1.701 / 1.690$ Å; they are slightly longer as expected for an AsO₄ tetrahedron: the substitution by Mo increases the bond distance whereas the small amount of P decreases the bond distance. The observed value contributes to this mixed occupation. Solid solution for the central atoms of these two tetrahedra is indicated by the analysis of the principal mean square displacements of the anisotropic displacement parameters: The O atoms involved in the X3O₄ and the X4O₄ tetrahedra exhibit stronger anisotropies as compared to all the other atoms. Especially the anisotropies of the central atoms X3 and X4 are in the same range as those of the Mo1 and Mo2 atoms. - The crystal structure is characterised by the connection of Bi2, Bi3, Bi4, and oxo-oxygen atoms to ribbons running parallel to [100]. These ribbons are linked via the second coordination sphere of their Bi atoms to the XO₄ tetrahedra and to the Bi1 atoms.