selenium crystals has a decisive effect on the evolution of their shape as the crystals grow in amorphous films.

Keywords: selenium-1, crystals-2, crystal shape-3

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Lomonosov State Academy of Fine Chemical Technology, Moscow, Russia. 

The different space group (sp. gr. I23 or sp. gr. P23) of crystals (a structure dissymmetrization) is attributed to the kinetic phase transition of order-disorder type. The causes are associated with a presence of several atoms in M position of sillenite structure and preparation conditions simultaneously.

1. Bii) or Bi24[M3+]O40 (M=Mn, V) and Bi24[Si2-yMy]O40 (M=Mn, V) have been synthesized in air, but neither crystal structures nor cell parameters were reported [2]. During phase investigations in the Li-Cu-B-O system we have found some new complex borates at ambient pressure, namely Li3CuB2O5, Li4CuB2O5, and a new polymorphic modification of CuB2O4 [3].


Institute for Complex Materials, IFW Dresden, Germany. Institute for Materials Science, Technische Universität Darmstadt, Germany. Institute for Inorganic Chemistry SB Russian Academy of Science, Russia. E-mail: d.mikhailova@ifw-dresden.de

Li-containing borates with 3d elements attract a large interest in the last years as potential intercalation electrode materials for Li batteries. For example, LiFeBO3 with chains of distorted edge-shared FeO3-units with Fe5+ [1], was proposed as a perspective cathode material for Li- insertion [1]. The advantages of such materials are an existence of 3d metals in different oxidation states and the ability of boron to form BO4-triangles and BO3-tetrahedra, which are connected with each other in a different manner.

The common feature of all known copper(I) borates is a Jahn-Teller distortion of Cu2+ coordinated polyhedra due to the electronic configuration of the d9 ion, which can lead to an anisotropic character of the crystal structure. The information about phases in the Li-Cu-B-O system is deficient and contradictory: three compounds Li3CuB2O5, Li4CuB2O5 and Li2Cu2O5 are synthesized in air, but neither crystal structures nor cell parameters were reported [2]. During phase investigations in the Li-Cu-B-O system we have found some new complex borates at ambient pressure, namely Li3CuB2O5, Li4CuB2O5, and a new polymorphic modification of CuB2O4 [3]. This new CuB2O4-polymer with a pseudo-layered monoclinic structure has both BO3-triangles and BO4-units consisting of corner-sharing BO3-triangles and BO2-tetrahedra. In contrast to the well-known triclinic form of CuB2O4 [4], layers are linked with each other by BO2-tetrahedra. Crystal structures of Li3CuB2O5 and Li4CuB2O5 exhibit only BO3 triangles, which are connected with each other via corners. LiCuB2O4 demonstrates infinite CuO-chains from CuO4-units consisting of edge-sharing CuO2-pyramids. These chains are responsible for the strong anisotropic character of the thermal expansion of the phase along the a-axis. In the structure of Li3CuB2O5, CuO2-octahedra and CuO2-pyramids can be identified with CuO bonds smaller or equal to 2.7 Å, which are connected with each other in a different manner.

Keywords: sillenites, composition, structure

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Keywords: Jahn-Teller distortion of Cu(II), layered structure, anisotropic thermal expansion

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Crystallographic Orientation Relationship between Bastnaesite, Fluocerite and Cerianite in a Single Crystal from the Pikes Peak Pegmatites. Mathis M. Müller, Hans-Joachim Klebe. GeoScience, Technical University Darmstadt, Germany. E-mail: mueller@geo.tu-darmstadt.de

A fluocerite (Ce,La)F3 single crystal intergrown with bastnaesite (Ce,La)(CO3)F from the Pikes Peak area in Colorado, USA was prepared for the investigation of the crystallographic orientation relationship between the two mineral phases via transmission electron microscopy. The epitactical overgrowth of bastnaesite on fluocerite was confirmed by evaluating the electron diffraction patterns of the relevant mineral phases. During the examination, a third mineral phase, which was unexpected in this phase relationship, was encountered mineral assemblage of bastnaesite, fluocerite and cerianite. The orientation matrix and the direction-plane relation for the three mineral phases was established.

Keywords: bastnaesite, orientation relationship, orientation matrix

FA2-MS16-P43

Ordering in intercalated Co atoms and electron density distributions of layered compounds CoTiS2. Ken-ichi Ohshima, Takuro Kawasaki, Miwako Takahashi Institute of Materials Science, University of Tsukuba, Tsukuba305-8573, Japan. E-mail: ohshima@bk.tsukuba.ac.jp

A structural study of layered compounds CoTiS2 (x=0.26, 0.43, and 0.57) by X-ray diffraction analysis was performed to investigate both the ordered atomic arrangement and disordering behavior of intercalated Co atoms, and the nature of the chemical bond from the electron density distribution (EDD) obtained by the maximum entropy method. The 2ax2ax2c superstructure of the Co atoms is observed for x=0.26 and 0.57, and disappears at 510 and 550K, respectively. On the other hand, 3ax3ax2c superstructure of the Co atoms is observed for x=0.43, and disappears at 610 K. It is understood that the type of the transition is second-order-like. The overlapping of the EDD between Co and S atoms & Ti and S atoms are clearly seen, which are corresponding to the covalent bonding in the van der Waals gap layer and in the TiS2 one. It is expected that nature of covalent bonding between Co and S atoms causes decreasing of the interlaye distance.

Keywords: layered compounds, ordering of the Co atoms, EDD

FA2-MS16-P44

Structural trends in the (emim)3[Mo6O26]3− (emim = 1-ethyl-3-methylimidazolium) group of compound. Anna Pakhomova, Sergey Krivovichev. Saint-Petersburg State University, Russian Federation. E-mail: a.s.pakhomova@mail.ru

Polypolymetalates (POMs) have many properties that make them attractive for applications in medicine, biology, magnetism, materials science and catalysis. POMs are a kind of competent structure-tunable building block because they exhibit a wide variety of structural motifs of different sizes and topologies. As far as we know, all known octamolybdates has been synthesized by hydro- and solvothermal methods. To the best of our knowledge, ionothermal methods were not used, although they recently have shown high promise in the preparation of novel metal-organic frameworks. We have used ionic liquid (emim)Br (emim=1-ethyl-3-methylimidazolium) as both solvent and template for the purpose of construction of novel organic-inorganic polyoxomolybdates of alkali metals. The three novel octamolybdates (emim)3K(Mo8O26) (1), (emim)3Rb(Mo8O26) (2) and (emim)3Cs2(Mo8O26) (3) (emim = 1-ethyl-3-methylimidazolium) have been obtained in the ionothermal reactions. The structures of these compounds are described on the basis of octamolybdate anions [{Mo6O26}3−]. In compounds 1 and 2, [{Mo6O26}3−] units are linked by metal cations to form chain structures, while Cs cations in the compound 3 link to polyoxoanions to form layer structure. This work was supported by a President of the Russian Federation Grant for Young Doctors of Science (to SVK, grant No. MD-407.2009.5).

Keywords: ionothermal synthesis, alkali polyoxomolybdates, X-Ray crystal structure determination

FA2-MS16-P45


High-pressure cells reduce significantly the accessible reciprocal space in single-crystal studies and, moreover, the parts of cells traversed by radiation produce as a rule strong background features. In order to increase the quality of measured data and accuracy of calculated structural parameters it is of primary importance to reduce these deleterious effects. In Diamond Anvil Cells (DAC) diamond anvils must be supported by a strong and X-ray transparent...