FA2-MS16-P10

Crystal Chemistry of SnX-PbX (X=S, Se) mixed crystals.

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The systems SnS-(Pb,Sn)S; $SnS_{0,75}Se_{0,25}$-$(Pb,Sn)S_{0,75}Se_{0,25}$, $SnS_{0,5}Se_{0,5}$-$(Pb,Sn)S_{0,5}Se_{0,5}$ and $SnS_{0,25}Se_{0,75}$-$(Pb,Sn)S_{0,25}Se_{0,75}$ were investigated to determine the regions where solid solutions exist. There the crystals have orthorhombic structure. The miscibility gaps have been determined by electron microprobe analysis and X-ray powder diffraction.

The samples were synthesized by solid state reaction in closed silica ampoules. The width of solid solution range, i.e. the Pb/Sn-ratio too, depends strongly on the S/Se-ratio. The lattice parameters of the orthorhombic phases were determined by X-ray powder diffraction. To grow single crystals via chemical vapour transport this powder was used as source material. Iodine acts as transporting agent. These single crystals should have a good electrical conductivity similar to SnS-(Pb,Sn)S films grown by vacuum evaporation [1].

[1] K. Bente, V. V. Lazenka, D. M. Unuchak, G. Wagner, and V. F. Gremenok, Cryst. Res. Technol. 45, No. 6, 643 – 646 (2010) / DOI 10.1002

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FA2-MS16-P11

Dense packing of identical ellipses with 6 contacting neighbours.

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For the densest packings of ellipsoids and ellipses, Matsumoto and Nowacki first discussed and derived 13 and 2 different densest packings of ellipsoids and ellipses respectively[1]. They assumed that the densest packings are only those which result from the closest packings of spheres (ccp and hcp) and circles by an affine transformation respectively.The packing density and the contact number of these packings for ellipsoids are $\rho = \pi/3\sqrt{2}$=0.74048.., and N=12, the same as the ccp or hcp. And the density of derived packings of ellipses is $\rho = \pi/2\sqrt{3}$=0.906899.., and the contact number is N=6. Moreover, they are all homogeneous packings, namely all ellipsoids or ellipses , are crystallographically equivalent.

There are 7 dense homogeneous packings of ellipses with 6 contacting neighbours [2],[3]. Among them, 2 types of *p2* and *c2mm* attain the maximum density, 0.906899 being the same of the closest packing of circles,*p6mm* [1]. The *p2gg-2a2* packing cannot attain the maximum density [4].

Since 1992, Tanemura and Matsumoto have presented the proof, with the aid of computer, that the other 3 types of packings of ellipses, *p31m, p3,* and *p2gg 4c1(I),*cannot exceed the maximum density of circles [5],[6] and [7]. The packing density depends on axial ratio *k=a/b* for *p31m*, and a tilt angle θ of major axis together with the shape parameter *k=a/b* for *p3,* and *p2gg 4c1(I)*. The other *p2gg 4c1(II)* packing of ellipses also shows no maximum density and is composed of *p2* and *p2gg-2a2* regions. The packing density is the function of the shape parameter *k=a/b* and the tilting angle θ [8],[9].

Concerning the dense packings of ellipsoids and ellipses, superdense crystal packings of ellipsoids have been reported [10]. Even though we cannot understand these packings, the contradict packings of ellipses with the hypothese in [1], are not found.

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Keywords: packings of ellipses and ellipsoids; dense packings; homogeneous packings

FA2-MS16-P12

Structure and Energetics of the FeOOH Polymorphs and their Surfaces from First Principles.

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Iron oxyhydroxides (FeOOH) play an important role in a series of environmental and technological processes, e.g. in binding heavy metals. Using density functional theory (DFT), we study the bulk properties of the FeOOH polymorphs goethite (□), akaganeite (□), lepidocrocite (□), and the high-pressure phase□) at ambient conditions and under hydrostatic pressure. The energetic relations among the phases reveal that the framework structures□□( ) are more favorable than the layered one (□) [1]. Moreover, we explore the stabilization of akaganeite by filling the large 2x2 channels with ions such as Cl^-, SO_4^{2-} or AsO_4^{2-}. The FeOOH polymorphs have high surface areas and high adsorption affinities for aqueous solutes [2]. Therefore, we analyze structural, energetic, and sorption properties of the bare and hydroxylated goethite(101), akaganeite(100), and lepidocrocite(010) surfaces.

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FA2-MS16-P13

Crystal structure solution of the mineral sanjuanite from laboratory powder diffraction data.

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