the trigonal phase R-3m at a temperature \( \approx 457 \) K [1], corresponding to behaviour of dielectric and optical properties. The trigonal phase exists in a very narrow temperature interval in comparison with isostructural \( M_2H(XO_3)_2 \) crystals [2]. The obtained structural data confirmed the previously proposed mechanism of conduction in crystals of this family: the appearance of a high protonic conductivity is associated with the formation of a qualitatively new system of hydrogen bonds - the dynamically disordered hydrogen bond network, in which both the proton positions in hydrogen bonds and the bond orientations are dynamically disordered. The network of hydrogen bonds thus formed enables protons to move over vacant crystallographically equivalent positions, which leads to anomalously high hydrogen diffusion coefficients and to superionic conductivity. Also it was received the information about solid state reactions (the crystalline state remains), occurring in investigated crystals with an increase in the temperature. The temperature increase above the trigonal phase leads to formation of \( K_2SiO_3 \) phases in the samples under study. The heating and cooling of the samples lead to formation of \( K_2SiO_3 \) phases also. It is necessary to notice, that according to the powder data there are absent diffraction peaks corresponding to \( KH_2SiO_3 \) compound, which could be formed in \( K_2(HSO_4)_2 \) samples in the process of solid state reactions, as it is supposed under the literary data. The formation of a multiphase state is confirmed by X-ray diffraction data, scanning electronic microscopy and the energy dispersive X-ray spectroscopy.

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Keywords: crystal and powder X-ray diffraction structure analysis, phase transitions and structure, superionic conductivity

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Y\(_3\)H\(_2\)Si\(_4\)O\(_8\): A naturally occurring defect silicate of the KDP-structure type. Thomas Malcherek\(^a\), Jochen Schlüter\(^a\), Boriana Mihailova\(^b\), Tomas A. Husdal\(^c\).

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A new type of rare earth (RE) silicate with idealized composition \((Y, Ln)\)_2H\(_2\)Si\(_4\)O\(_8\) (Ln = Gd, Tb, Dy, Ho, Er, Yb) (YSO) has been identified in a granitic pegmatite of the I-42d class. The obtained crystallographic data have been collected on several single crystals of YSO. The structure refinements on average yield Si-occupancies of 75±5%. The presence of heavy RE elements on the Y-site has been modelled using the Yb scattering factor curve, resulting in Yb/Y ratios of 1/4. Similar compositions are obtained by electron microprobe analysis, also indicating the presence of other heavy RE cations. Raman microspectroscopy performed on the crystals used for the X-ray structure analysis, confirms the presence of OH-stretching modes. The crystal chemistry of the new compound and possible similarities to KDP in terms of hydrogen bonding are discussed.


Keywords: hydrogen bonding of minerals, rare-earth compounds, ferroelectrics and related materials

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Evolution of the Shape of Nanothin Selenium Crystals during their Growth in Amorphous Films. Malkov Andrey\(^a\), Malkov Vyacheslav\(^b\), Stekalovsky Victor\(^c\), Malkov Oleg\(^d\), Puchin Vladimir\(^e\), \(^a\)Institute of High-Temperature Electrochemistry, Ural Division RAS, \(^b\)“ROSNA” Scientific and Production Center, \(^c\)Institute of Metal Physics, UD RAS, Ekaterinburg, Russia.

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The method of transmission electron microscopy was used to study the evolution of a rotational distortion of the lattice and the shape of nanothin (80÷100 nm) crystals of hexagonal selenium growing in amorphous films at crystallization temperatures of 180–120°C. It was found that the lattice of nanothin selenium crystals growing in amorphous films at crystallization temperatures of 180–150°C undergoes a nonuniform elastic rotational distortion around the [001] direction (180÷160°C) or in two mutually perpendicular directions, namely, around [001] and the perpendicular direction of the maximum growth rate (150°C). Nanothin selenium crystals growing in this range of crystallization temperatures have a rectilinear rhombic shape (Fig.1a,b). At crystallization temperatures of 140÷120°C the lattice of nanothin selenium crystals undergoes a nonuniform elastoplastic rotational distortion around three mutually perpendicular directions [1]. In addition to the aforementioned directions, the lattice of nanothin selenium crystals undergoes a nonuniform rotational distortion around a direction, which is not in the film plane and is perpendicular to the first two directions. It is called an azimuthal distortion. The nanothin selenium crystals, which grow at crystallization temperatures of 140÷120°C, have a distorted curvilinear rhombic shape (Fig.1c,d). The sign of distortion of the shape of a nanothin selenium crystal always coincides with the sign of the azimuthal distortion of its lattice (Fig.1c,d). It can be concluded from this fact that the azimuthal distortion of the lattice of a nanothin selenium crystal determines the azimuthal distortion of its shape.

Fig. 1. Evolution of the shape of nanothin selenium crystals: rhombohedral crystals of a rhombic shape (a, b); nanothin crystals of a curvilinear shape (c, d), ×10 000

A model for the evolution of the shape of nanothin selenium crystals has been proposed. This model is based on the assumption that the evolution of the real structure of nanothin...