can be used to perform a two-phase refinement using Jana2006 [6]. Furthermore, domains of the two phases were observed by HT high-resolution transmission electron microscopy (TEM) and dark field TEM. The aluminium end-member $Ca_2Al_2O_5$ shows an isotypic incommensurate structure above 1075(10)K.

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Keywords: incommensurate phases, high-temperature structures, TEM

P10.05.26

T, 2T and 4T wollastonites derived by the Ge substitution

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Four kinds of structures of wollastonite whose compositions were $CaGeO_3$, $Ca(Ge_{0.65}, Si_{0.35})O_3$, $Ca(Ge_{0.50}, Si_{0.50})O_3$ and $Ca(Ge_{0.15}, Si_{0.85})O_3$ were studied. They are called 100Wo, 65Wo, 50Wo and 15Wo, respectively. The lattice constants of 100Wo, 65Wo, 50Wo and 15Wo are: (angstrom, degree) a=8.125(2), 2X8.038(4), 2X7.995(2), 4X7.949(5), b=7.554(1), 7.451(1), 7.400(1), 7.352(1), c=7.292(2), 7.194(2), 7.148(2), 7.093(1), alpha= 90.11(3), 89.93(2), 90.05(2), 90.06(2), beta=94.40(3), 94.85(2), 94.97(2), 95.11(1), gamma=103.48(1), 103.34(2), 103.43(1), 103.39(1), respectively. 100Wo shows the basic-wollastonite. 65Wo consists of the neighbouring two units of the basic-wollastonite along the a-axis. The X-ray diffraction pattern showed a pseudo-C lattice. Therefore, the stacking sequence of 65Wo can be represented as AB, where A is the unit cell of the basic-wollastonite and B is the unit cell of the basic-wollastonite with $b/2$ displacement. 50Wo consists of the neighbouring two units of the basic-wollastonite along the a-axis, too. However, the X-ray diffraction pattern was different from 65Wo. Judging from the X-ray diffraction, the stacking sequence of 50Wo is represented as AA. 15Wo consists of the four units of the basic-wollastonite along the a-axis. There were four possible stacking sequences: AAAA, ABAB, AABB and AAAB. The structure having the sequence AAAA will show the strong intensity on the h=4n diffraction. The structure ABAB will show the strong intensity on the h=2n diffraction. The structure AABB will show the extinction rule of the pseudo-C lattice. The last structure AAAB will not show any characteristic rules. As the result of the observation of the X-ray diffraction of 15Wo, it was clear that the stacking sequence AAAA was most reasonable.

Keywords: germanates, crystal structure determination, superstructures

P10.05.27

Description of modular minerals within the superspace approach

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Modular structures are frequently observed in the mineral world. These structures are built of modules, approximately described by simpler structures. The Pb-Bi-Ag sulphosalts of the lillianite homologous series are examples of modular minerals based on PbS-like structure. The fact that the structure of these minerals can be described with the help of a simple average structure in combination with additional small distortions moved us to explore the potential of the so-called superspace approach for their description. The superspace formalism was originally developed for the study of modulated structures and is by now a well established tool for the treatment of incommensurately modulated structures, composite crystals or quasicrystals. But superspace is also a powerful and efficient tool for dealing with the structural properties of commensurate systems with large unit cells. A necessary condition is that the structures have approximate much smaller subperiodicities, which is the case for modular structures. The superspace formalism allows a unified description of whole homologous series, with the number of structural parameters smaller than in a conventional approach, and predicts the observed three dimensional space groups of individual members. With the introduction of some new concepts we have successfully applied the superspace method to the analysis and refinement of the lillianite homologues. The structures are best described as modulated structures, but with unusually large displacive modulations of a linear "zig-zag" type. An efficient treatment required the modification of the refinement program JANA2006 in order to introduce this type of functions as alternative basic modulations.

Keywords: modular structures, superspace approach, lillianite homologous series

P10.05.28

Polytypism in cronstedtite

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Cronstedtite is a trioctahedral 1:1 phyllosilicate, with iron and silicon as major cations. It occurs in low- and medium- tempered hydrothermal deposits and in some kinds of meteorites. Its structure is composed of the octahedral (Oc) and tetrahedral (Tet) sheets forming the 1:1 layer by sharing apical oxygen atoms. All octahedral positions are fully occupied by Fe^{2+} and Fe^{3+}; the Si atoms in tetrahedra are partially replaced by Fe^{3+}. The layers are linked together mainly by hydrogen bonds. The polytypes of cronstedtite are divided into

four Bailey's groups (or OD subfamilies) termed A, B, C, and D, according to shifts and rotations of consecutive layers: +-ai/3 shifts for group A, +-ai/3 shifts and 180 degrees rotation for group B, +-b/3 or zero shift for group C, +-b/3 or zero shifts and 180 deg. rotation for group D, where ai and b correspond to the edges of hexagonal and orthohexagonal cells, respectively. The ordered polytypes are represented by regular sequences of shifts and/or rotations allowed by the stacking rule of the respective subfamily. More or less disordered crystals are common. Recently, crystal structures of polytypes of cronstedtite 3T, 1T, and 2H2, representing groups A, C, and D, respectively, were refined. No polytype in the group B has been found to date. Subfamilies and polytypes can be identified by following methods: (1) Single-crystal X-ray diffraction (XRD) (2) Selected area electron diffraction (SAED) (3) Electron back scattering diffraction (EBSD) (4) High resolution electron transmission microscopy (HRTEM) Refined structures, X-ray diffraction pattern, HRTEM, and SAED images of several polytypes are presented.

Keywords: layered silicates, HRTEM, single-crystal X-ray diffraction

P10.05.29

New NaAlSiO₄ polymorphs: Monoclinic and orthorhombic trinepheline

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Recently, a new structural variety of nepheline with composition $Na_{7.85}Al_{7.85}Si_{8.15}O_{32}$ was obtained by single crystal growth experiments using a cryolite flux. It crystallizes in space group $P112_1$, a = 9.9897(6) Å, b = 9.9622(6) Å, c = 24.979(2) Å, γ = 119.788(4)°, Z = 3. The crystal structure of monoclinic trinepheline can be explained as a stacking sequence of a conventional nepheline unit cell and one additional layer built exclusively of elliptical rings, as observed in the structure of hexagonal trinepheline. When heated to 373(5) K, monoclinic trinepheline transformed to trinepheline of hexagonal symmetry (space group $P6_1$). Upon further heating at 473(5) K the crystal structure corresponds to that of conventional nepheline. Furthermore, we have determined the structure of an orthorhombic polymorph of NaAlSiO₄ ($Pna2_1$, Z = 36), which was hydrothermally synthesized and described by Klaska in 1974 (Thesis, University of Hamburg). The lattice parameters are related to the $P6_3$ ones through the relationship a(ortho) ≈ sqrt(3)/2 * a(hex) ≈ 8.66 Å; b(ortho) ≈ 1.5 * a(hex) ≈ 14.94 Å; c(ortho) ≈ c(hex) ≈ 25.14 Å. The crystals were affected by twinning via the sixfold axis. This polymorph is built of the elliptical rings and the resulting layers are comparable to the ones in hexagonal trinepheline. In hexagonal trinepheline, however, the neighbouring layers are rotated with respect to each other. In the orthorhombic modification, the layers are stacked on top of each other in identical orientations. We will also present some results of an *ab-initio* study on Na nepheline (known for showing Na-solid state conductivity) performed within the DFT formalism as implemented in the SIESTA code.

Keywords: single-crystal growth, single-crystal structure analysis, *ab-initio* calculations

P10.05.30

Hydrogen positions in beryllate minerals and materials by combined X-ray and neutron diffraction

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For mineral systems information on their structure, including the localisation of light atoms such as hydrogen and beryllium, is of considerable importance as it allows a better understanding of the material behaviour under natural conditions including its paragenesis, phase stability, compressibility/water content and thermal expansion. Many important natural minerals and their analogues are not simple silicates or aluminosilicates, but also incorporate other framework forming species such as the beryllate tetrahedron, BeO_4. The role of the hydrogen containing species such as H_2O and OH is also central to determining the structure formed and distribution of non-framework species in the material. We have found that the optimised crystallographic method of determining the full crystal structures of these minerals, including accurate hydrogen positions and framework distributions of Si, Al and Be, is a combined single crystal X-ray - powder neutron diffraction method. Powder neutron diffraction data are collected on the hydrogenous natural material at 120 K and the data analysis simultaneously fits this and the SXD (single-crystal X-ray) data collected at the same temperature. In the presented study the following minerals have been investigated and detailed structures will be presented: 1) Eudidymite and Epididymite. Differences in these compositionally identical minerals, $NaHBeSi_3O_8$, have been determined and results from the orientation of an extra framework hydroxide anion. 2) Leifite $Na_2(Si,Al,Be)_7(O,OH,F)_{14}$. 3) Sorensenite $Na_4SnBe_2Si_6O_{18}$ 2 H_2O. 4) Nabesite $Na_2BeSi_4O_{10}$ 4 H_2O. 5) Semenovite $(Na,Ca)_9(Ce,La)_2(Fe^{2+},Mn)(Si,Be)_{20}(O,OH,F)_{48}$.

Keywords: combined X-ray - neutron diffraction, beryllates, hydrogen positions

P10.05.31

Structural features of the M-site vacancies and possible hydrogen positions in hydrous forsterite

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The result of the structural refinement [1] of synthetic Fe-bearing hydrous forsterite synthesized at 13.5 GPa and 1400℃ [2] revealed that the cation vacancies at the octahedral M sites predominantly occur at the M2 site, in contrast to the case [3][4] of Fe-free hydrous forsterite synthesized at 13.5 GPa and 1300℃ [5] revealed that the cation vacancies at the octahedral M sites predominantly occur at the M1 site. In the case of Fe-free hydrous forsterite, the structural strain from the ideal size is larger in M1 site than in M2 site. Two H atoms may replace the Mg atom predominantly at the M1 site to reduce the structural strain, giving the vacancy at the M1 site. In the case of Fe-bearing hydrous forsterite, the Fe atoms occupy both M1 and M2 sites, leading the combinations of Mg-Mg, Fe-Fe, Mg-Fe and Fe-Mg for the occupation of M1-M2 sites. Among these, the combination of Fe-Mg for M1-M2 sites may have maximum structural strain from