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

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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

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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

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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