

triangles. Sheet f is composed of [9]-coordinated (Ca,REE, Y) polyhedra, Si tetrahedra and B triangles. In sheet g, [6]-coordinated sites are 67% occupied by Ti and Nb, and B triangles are only 17% occupied by B. In sheet h, [6]-coordinated sites are only 17% occupied by Ti, they are coordinated by OH and H<sub>2</sub>O groups. Two identical h sheets are connected via common vertices of 17% occupied Ti octahedra which are H<sub>2</sub>O groups. In sheet k, the [8]-coordinated sites are 22% occupied by Ba. The structure is a framework of cation polyhedra which can be considered an intercalation of three domains: one fully ordered with full occupancy of cation sites, and two partly ordered with cation-site occupancies of 67% and 17%, respectively. To acknowledge the extreme chemical and structural complexity of this mineral, we chose the name byzantievite. "Byzantine" means "intricately involved". For 12 centuries (374-1453), the Byzantine Empire was home to many different peoples and religions. The structure of the Empire was extremely complex but the state functioned very efficiently, and shaped Europe and modern civilization.

**Keywords:** byzantievite; framework; new mineral

#### FA2-MS01-O6

**A Few Applications of the Superspace Approach in Mineralogy.** Alla Arakcheeva. *Laboratoire de Cristallographie, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland.*

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It is fair to claim that the development of crystallography was initiated by mineralogy. First the crystal forms and later crystal structure determinations did primarily instigated the mathematical description of minerals. Crystal chemistry is essentially based on the large amount of structure determinations of natural minerals. It is not surprising that precisely the minerals natrite, Na<sub>2</sub>CO<sub>3</sub> [1] and calaverite [2] have played a fundamental role in the development of the superspace theory. Currently, the superspace concept is successfully applied for the determination and description of a many incommensurately modulated crystal structures (IMCS) including minerals. For example, investigations of minerals like fresnoite, melilite, laszurite, akermanite, sartorite, labradorite, srebrodolskite, tridymite, quartz (between  $\alpha$  and  $\beta$  modifications) could only be meaningful with the superspace symmetry approach. The IMCSs of minerals give the possibility to study details of their crystal chemistry, which can be used for a better understanding of their genesis. For instance, the determination of IMCSs in the calaverite-sylvanite group, Au<sub>1-x</sub>Ag<sub>x</sub>Te<sub>2</sub>, [2, 3] reveals different degrees of valence fluctuations on the Au-position, which are due to different degree of the Ag ordering on the Au position. The IMCSs of two different occurrences of natrites allow to distinguish specific characteristics of Na and CO<sub>3</sub>, although their average structures are identical. In material science, mineral names are used to characterize of structure types. With the superspace approach, the structure type (ST) concept can be generalised in (3+1)D symmetry space [4] (3+1)D ST can be used not only to predict 3D structures but also to identify them [4]. In addition to the

pioneering scheelite (3+1)D ST [4], the calaverite (3+1)D ST [3] is able to characterize calaverite, sylvanite, kostovite and krennerite minerals as well as NbTe<sub>2</sub>, TaTe<sub>2</sub>, VTe<sub>2</sub>, synthetic compounds based on the unique *C2/m*( $\alpha 0\gamma$ )(0s) superspace group with identical basic structures. The (3+1) D ST concept permits also a unified symmetry approach for group-subgroup considerations in phase transitions [5]. The superspace approach born from the study of mineralogical samples now is an effective tool, which can be applied to the needs of mineralogy. The precise characterization of isomorphic substitution is greatly facilitated with IMCSs determination. Investigation of IMCSs allows to predict series of 3D structures and, sometimes, polymorphic modifications [6]. The extension of the ST concept in (3+1) D space appears to be an effective way to identify structure-relation properties.

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**Keywords:** mineralogy and crystallography; incommensurately modulated structures; classification of crystal structures

#### FA2-MS01-O7

**Cr<sub>x</sub>Re<sub>1-x</sub>O<sub>2</sub> Oxides with Different Rutile-like Structures: Changes in the Electronic Configuration and Resulting Physical Properties.**

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Rutile type crystal structures and their derivatives are based on the same topology: straight chains of edge-sharing MO<sub>6</sub> octahedra for the cations M are connected via corner-sharing to four surrounding chains [1]. Rutile-derivatives show ordering of cations, anions or distortions of coordination polyhedra.

Several complex oxides of Cr<sup>3+</sup> with rutile, trirutile or rutile-like structure exist, because the ionic radius of Cr<sup>3+</sup> (0.62 Å) is close to the one of Ti<sup>4+</sup> (0.61 Å) for octahedral oxygen coordination. Ternary oxides in the system Cr – Re – O are less intensively investigated, although these systems offer an additional degree of freedom due to the ability of the Re ion to adopt formal oxidation states between +4 and +7 in complex oxides with different resulting properties. Both end members, CrO<sub>2</sub> [2] and the monoclinic modification of ReO<sub>2</sub> [3], have a rutile-like structure.

In our work [4], mixed chromium-rhenium oxides, Cr<sub>x</sub>Re<sub>1-x</sub>O<sub>2</sub> with 0.31 ≤ x ≤ 0.66, have been synthesized for the first time by high-pressure high-temperature synthesis and