

MS15-03 From calcite to the first natural hexaniobate or 350 years of mineral science. Henrik Friis,^{ab} ^aMineral Deposit Research Unit, Department of Earth & Ocean Sciences, University of British Columbia, 6339 Stores Road, Vancouver, BC, V6T 1Z4 Canada, ^bNatural History Museum, University of Oslo, P.O. Box 1172, Blindern, 0318 Oslo, Norway
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Scandinavia has in many ways been the birthplace of modern crystallography and material science. The pioneers of these sciences did their work on natural occurring minerals more than 350 years ago, and two of these were the Danes (Nils Stensen or Nicholous Steno and Rasmus Bartholin or Erasmus). Steno studied quartz and found that the angles between corresponding faces were consistent between different quartz crystals although the actual faces varied [1]. This was the first basis for crystallography and is now known as Steno's Law. The same year Bartholin published his observations of birefringence in exceptionally clear calcite from Iceland known as 'Iceland Spar' [2]. The diverse geology of the Scandinavian countries results in numerous exceptional mineral occurrences containing minerals with unique structures. Furthermore, natural minerals are rarely pure compounds, i.e. they can contribute to the understanding of structural compensation through increasing trace element (dopant) level. The first polyoxometalate (a molybdate) was described by the Swedish chemist Jöns J. Berzelius in 1826 [3]. Despite a large number of polyoxometalates not much work has been carried out on polyoxoniobates [4]. Only two natural polyoxoniobates have been found and both are heteropolyniobate, namely menezesite ($\text{Ba}_2\text{MgZr}_4(\text{BaNb}_{12}\text{O}_{42})\cdot 12\text{H}_2\text{O}$) [5] and aspedamite ($([\text{Nb}_2\text{Fe}_2^{7+}\text{Fe}^{5+}]\text{Nb}_4(\text{ThNb}_9\text{Fe}_2^{7+}\text{TiO}_2)(\text{OH})_3\cdot 9\text{H}_2\text{O})$) [6], the latter is described from Norway. Here the first natural hexaniobate will be presented, which was also found in Norway. The mineral contains two Nb-sites forming the well-known $[\text{Nb}_6\text{O}_{19}]^{8-}$ Lindqvist ion [7]. Four Nb1 octahedra are each edge sharing with two other Nb1 octahedra in the same plane forming a quadrate. Above and below the centre of the quadrate two Nb2 octahedra are edge sharing with all four Nb1 octahedra forming a super octahedron. The Lindqvist ions are interconnected by corner and edge sharing with Mn2+ octahedra forming a three dimensional structure. Two Mn1-octahedra are edge sharing on one Lindqvist ion in a trans-configuration. Each of these sites is connected to two different Lindqvist ions through bridging oxygens. The Mn2 octahedra are attached to the terminal oxygen of the Nb2 octahedron. The ideal formula of the mineral is $\text{Mn}_4\text{Nb}_6\text{O}_{19}\cdot 14\text{H}_2\text{O}$. One of the waters is found as crystal water in channels, the rest are attached to the terminal oxygens of the Mn octahedra. The second part of the paper deals with the structural affect of incorporating foreign elements, especially Rare Earth Elements (REE), into natural minerals, and how this knowledge can be transferred to synthetic compounds. This would be applied to luminescent minerals and compounds. The main phases discussed will be fluorapatites, zeolites and related structures.

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MS15-04 Crystallography of shadows: local disorder in intermetallic compounds. Yuri Grin,^a Yurii Prots,^a Horst Borrmann,^a ^aMax-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany
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The development of the knowledge on intermetallic compounds, the understanding of their chemical nature is still not complete. The coordination of atoms in their crystal structures is difficult to describe by means of traditional MO pictures as well as by means of the free-electron-gas model. On the other hand, the chemical and physical behaviour of this group of materials may be understood only taking in account the real atomic arrangements in the crystal structures.

Recent investigations of the crystal structures of the intermetallic compounds applying the advanced diffraction techniques reveal often new structural features which are hardly detectable by standard experiments. In particular, by careful analysis of the residual electron density different kinds of structural disorder were observed appearing in relatively small amounts [1]. Additional experimental proof is obtained by NMR [2] experiments and TEM studies [3,4].

In general this phenomenon appears as a presence of two different structural motifs – majority and minority one – existing within one single crystal. Such structural behaviors were observed in different groups of intermetallic compounds of rare-earth metals with main-group elements and transition metals, e.g. α - and β -modifications of TmAlB_4 [1,3,4] and rare-earth gallides $\text{Eu}_{3-x}\text{Ga}_{8+3x}$, $\text{Eu}_{1-x}\text{Ga}_{2+3x}$ [5], $\text{Sr}_{1-x}\text{Ga}_{2+3x}$ and $\text{Ca}_{1-x}\text{Ga}_{2+3x}$ [6,7], $\text{YbGa}_{2.63}$ [8] and $\text{Sr}_{3-x}\text{Ga}_{8+3x}$ with $x = 0.15$ [9]. The minority motif is either a tiling variant of the majority one or completely chemically different from the majority one. Requirements of chemical bonding may cause appearance of such atomic disorder and lead to unusual features in physical behavior.

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