INORGANIC CRYSTALLOGRAPHY AND GEOSCIENCES

Hatoyama, Japan. ^dDept. of Plant Anatomy, Eötvös University, Budapest, Hungary. E-mail: posfaim@almos.vein.hu

We have used a combination of advanced transmission electron microscopy techniques to study the physical and chemical properties of intracellular ferrimagnetic magnetite (Fe₃O₄) crystals inside magnetotactic bacteria collected from lakes and streams.

The orientations and morphologies of the crystals in a double magnetosome chain were identified using electron diffraction, high-resolution electron microscopy and high-angle annular dark field electron tomography. The chain is analogous to beads on a string, in which biological control appears to be stricter in setting the [111] magnetocrystalline easy axis of the crystals to be parallel to the chain axis than in constraining their orientation about this direction. We have used off-axis electron holography to record magnetic induction maps from the same particles. The magnetic signal is dominated by inter-particle interactions and by the shapes of the individual crystals.

We have also studied the diversity of magnetosomes in bacteria collected from Lake Balaton. In stained thin sections of cocci, magnetite crystals appear to be anchored to the inner cell membrane. They are enveloped by stained material, apparently representing the magnetosome membrane. The cells do not contain detectable iron outside the magnetite magnetosomes.

Keywords: biomineral, magnetism, advanced electron microscopy

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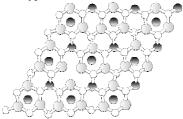
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Going Inside Fettelite, a Hg-Sulfosalt Mineral

Mónica Pérez-Priede^a, Xavier Xolans Huguet^b, Dámaso Moreiras Blanco^c, Santiago García Granda^a, ^aDepartment of Physical and Analytical Chemistry, University of Oviedo, Spain. ^bDepartment of Crystallography, Mineralogy and Mineral Deposits, University of Barcelona, Spain. ^cDepartment of Geology, University of Oviedo, Spain. E-mail: mpp@fq.uniovi.es

Fettelita's name honours Mr. M Fettel who found it. The empirical formula from microprobe analysis (based on 24 Ag atoms) is $Ag_{24}Hg$ $Cu_{0.04}Fe_{0.03}Tl_{0.02}Pb_{0.01}Sb_{0.07}As_{5.01}S_{20.07}$, ideally $Ag_{24}HgAs_5S_{20}$, and the crystal system trigonal [1].

Despite Fettelite sensitivity to X-Ray exposition, we have tried to elucidate its structure. As in Laffittite [2], metal and sulphur atoms form hexagonal rings linked by sharing their edges giving rise to parallel sheets when view along the c axis (see figure). The sheets join themselves composing a three dimensional network. Coordination around the metal ion is typical for sulfosalt structures.



[1] Wang N., Paniagua A., N. Jb. Miner. Mh., 1996, H. 7, 313-320. [2] Nakai I., Appleman D. E., American Mineralogist, 1983, **68**, 235-244.

Keywords: sulfosalts, mineral crystal structures, mineralogy and crystallography using X-ray diffraction

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Crystal Structure of Non-Metamict Minerals of Chevkinite Group Federica Liziero^a, Elena Belluso^b, Susanna Carbonin^a, Luca Nodari^c, Umberto Russo^c, ^aDip. Mineralogia e Petrologia, Univ. Padova. ^bDip. Sc. Mineralogiche e Petrologiche, Univ. Torino. ^cDip. Scienze Chimiche, Univ. Padova. E-mail: federica.liziero@unipd.it

Crystal chemistry and structure of chevkinites occurring in a high-temperature pneumatolitic vein from Tangir Valley (Pakistan) and in some silica-saturated/oversaturated syenite clasts from São Miguel Island (Azores) were investigated.

Electron microprobe analyses suite the formula $A_4BC_4O_8(Si_2O_7)_2$, where A = REE, Ca, Th; B = Fe, Mn, Mg; C = Ti, Fe, Nb. Ce and La

are the predominant elements in A sites: Ce₂O₃ range from 22% to 24% (wt.) and La₂O₃ from 10% to 14%. The major components in octahedral sites (B and C) are Fe and Ti: FeO range from 11% to 12% (wt.) and TiO₂ from 15% to 17%. The crystal structure was refined in the space group C2/m to conventional $R(I/\sigma(I)>4)$ of $\cong 2\%$. Site occupancies were calculated on the basis of electron microprobe results, refinement electrons and bond valence analysis. An $Fe^{3+}/\Sigma Fe$ ratio of 0.58 for Pakistan chevkinite was determined from Mössbauer spectroscopy. A preliminary spectral analysis points to the presence of two different types of Fe²⁺, both in octahedral sites. TEM investigations revealed the high crystallinity of both chevkinites. At the SAED scale the Pakistan chevkinite shows absence of structural defects, whereas the Azores one shows strekked spots along [001] and [-111] directions. HRTEM study is in progress in order to explain the presence of defects in some directions and to evidence structural regularity in others.

Keywords: silicates of rare elements, crystal chemistry and structure, TEM

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Structure of New Rare-Earth Borates $Ln[B_6O_9(OH)_3]$ and its Relation to Boracites

<u>Anna Ivanova</u>, Elena Belokoneva, Olga Dimitrova, Sergej Stefanovich, *Moscow State University, Moscow, Russia*. E-mail: an ivanova@mail.ru

The crystal structures of rare-earth borates $Ln[B_6O_9(OH)_3]$, Ln=Sm-Lu, synthesized under hydrothermal conditions, are solved in the space group R3c (Ln=Ho, a 8.385(9), c 20,71(4), R = 29%, and Ln=Gd, a 8.410(4), c 20,72(1), R = 4.8%). New borates belong to hexaborate group. The polar anionic framework consists of fundamental building blocks FBB [3T+3 Δ]: six-membered rings of regularly alternating (BO₄)-tetrahedra and (BO₃)-triangles. Atoms of Ln and H are located in wide channels along threefold axis. Ln-borates have the closest structural relation to synthetic boracite $Li_4B_7O_{12}Cl$ with the same FBB [1].

Structural relationship between all boracite modifications can be revealed, if to pay attention to clusters of four hexaborate blocks of two types [6T] or [3T+3 Δ]. In the cubic boracites $M_3B_7O_{13}Cl$ (M=Mg, Fe) [2] and many synthetic analogues four blocks [6T] are linked via vertices. The trigonal and orthorhombic distortion [3] is caused by increase one of B-O bond and corresponding decrease of B coordination from tetrahedron to triangle. In the cubic $Li_4B_7O_{12}Cl$ such clusters consist of four blocks [3T+3 Δ]. In the trigonal $Ln[B_6O_9(OH)_3]$, in comparison with $Li_4B_7O_{12}Cl$, there is one B-atom less, what leads to destruction of such clusters with keeping single six-membered rings.

[1] Jeitschko W., Bither T.A., Bierstedt P.E., *Acta Cryst.*, 1977, **B33**, 2767. [2] Sueno S., Clark J.R., Papike J.J., Konnert J.A., *Am. Mineral.*, 1973, **58**, 691. [3] Dowty E., Clark J.R., *Z. Kristallogr.*, 1973, **138**, 64.

Keywords: rare-earth borates, boracites, structural topology

P.10.06.2

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Zeolites Gismondine and Li-ABW under Pressure: Synchrotron XRPD and MD Simulations

Maria Cristina Betti^a, Ettore Fois^b, Aldo Gamba^b, Cinzia Medici^b, Simona Quartieri^c, Gloria Tabacchi^b, Giovanna Vezzalini^a, Stefano Zanardi^a, ^aDepartment of Earth Sciences, University of Modena and Reggio Emilia, Italy. ^bDSCA, University of Insubria, Como, Italy. ^cDepartment of Earth Sciences, University of Messina. E-mail: bmc@unimo.it

The response to compression of the zeolites gismondine and of LiABW were explored by synchrotron X-ray powder diffraction and ab-initio Molecular Dynamics simulations. Different pressure-transmitting media were used: silicon oil and propane-isopropane as non-penetrating media, and a water-methanol mixture as penetrating one. The applied pressure spans from room pressure to about 10 GPa. The data collection was performed at SNBL1 beamline at ESRF (Grenoble) using a wavelength of 0.7 Å and a MAR 345 (pixel size