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Keywords: ilmenites, X-ray absorption, phase composition

P10.05.41*Acta Cryst.* (2008). **A64**, C503**Low temperature structural distortions of brucite**Bryan C Chakoumakos¹, Antonio M. dos Santos¹, Juske Horita¹, Arthur J. Schultz²¹Oak Ridge National Laboratory, Neutron Scattering Science Division, P.O. Box 2008, bldg 7962, Oak Ridge, TN, 37831-6393, USA, ²Argonne National Laboratory, Argonne, IL 60439 USA, E-mail: kou@ornl.gov

Neutron powder diffraction studies of brucite, Mg(OD)₂, indicate subtle structural anomalies at 100K revealed by the temperature dependence of the anisotropic atomic displacement parameters (ADPs). Over the temperature interval 135K to 75K, the anisotropic ADP ellipsoid of the oxygen atom in the single D/H site model changes from prolate to oblate. The anisotropic ADPs of the D/H atom also exhibit anomalous temperature dependence below 135K. In addition, the alpha-angle, defined as the angle between the single-site DO bond and the split-site DO bond, decreases from 300K to 75K then increases at lower temperatures, and below 135K the thermal contraction of the octahedral layer thickness ceases. Additional understanding of this structural behavior is being sought from Raman spectroscopy and heat capacity measurements. The brucite layer is a fundamental building unit of a great variety of geologically important hydrous phyllosilicates, which include micas and clays. Brucite has P3barm1 space group symmetry with 3 atom positions all on 3-fold axes in the asymmetric unit. The Mg atom is at the origin, and the O and D/H atoms have variable z-coordinates. Typically, the D/H position is moved off from the three-fold axis into a fractionally occupied split-position to better accommodate the large ADP found in the single-site model. Oak Ridge National Laboratory is supported by the Division of Materials Sciences, U.S. D.O.E. (contract DE-AC05-00OR22725 with UT-Battelle, LLC).

Keywords: brucite, thermal expansion mechanism, neutron powder diffraction

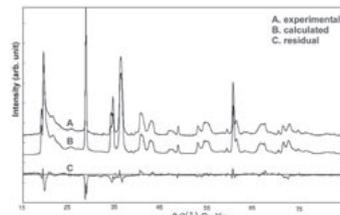
P10.05.42*Acta Cryst.* (2008). **A64**, C503**Simulation of powder XRD patterns from disordered phyllosilicates using information from HRTEM**

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Stacking disorder is a common phenomenon in phyllosilicates but its nature is difficult to be deduced using conventional diffraction techniques. In contrast, recent investigations using high-resolution transmission electron microscopy (HRTEM) have elucidated the structure of stacking disorder in various phyllosilicates, by directly observing individual layers and stacking sequences. Furthermore, simulations of X-ray diffraction (XRD) patterns using the information from the HRTEM results can complement the limited analysis area in TEM and quantify the density of the stacking disorder. In this paper, we describe several successful results to reproduce experimental powder XRD patterns from 2:1 phyllosilicates (pyrophyllite, talc, celadonite, etc.) including

considerable stacking disorder, using the DIFFaX program (Treacy et al., 1991) whose calculation parameters were derived from direct observation of stacking by HRTEM. The attached figure is an example of our results, comparison between the experimental and simulated patterns of disordered talc.



Keywords: stacking faults, high-resolution transmission electron microscopy, simulation X-ray diffraction

P10.05.43*Acta Cryst.* (2008). **A64**, C503**Rietveld and ⁵⁷Fe Mössbauer study of babingtonite from Shimane Peninsula, Japan**Masahide Akasaka¹, Takehiko Kimura¹, Mariko Nagashima²¹Shimane University, Geoscience, akasaka@riko.shimane-u.ac.jp, Matsue, Shimane Prefecture, 690-8504, Japan, ²University of Bern, mariko.nagashima@krist.unibe.ch, CH-3012 Bern Switzerland, E-mail: akasaka@riko.shimane-u.ac.jp

Oxidation state and distribution of Fe between two independent octahedral sites, Fe1 and Fe2, in babingtonite from Shimane Prefecture, Japan, were investigated using Rietveld and ⁵⁷Fe Mössbauer method. Babingtonite occurs in cavities of hydrothermally altered gabbro or dolerite, and is associated with prehnite and calcite. It is rhombic in form with edge length of 0.5-1 mm. This mineral has sector zoning, where Fe and Mn contents are different from each other, and compositional zonal structure with Mn and Al-rich core and Fe-rich rim. The chemical formula based on the average composition is (K_{0.004}Na_{0.006}Ca_{2.009})(Mg_{0.113}Mn_{0.094}Fe_{1.696}Ni_{0.02}V_{0.003}Cr_{0.001}Ti_{0.009}Al_{0.058})Si_{5.005}O₁₄(OH). The Fe²⁺:Fe³⁺-ratio based on the assumption that Fe1 and Fe2 sites are occupied by divalent and trivalent cations, respectively, is 45.2:54.8, which was consistent with the result by ⁵⁷Fe Mössbauer analysis: Fe²⁺:Fe³⁺-ratio determined from the area ratio of the doublets of Fe²⁺ (*IS* = 1.160 mm/s, *QS* = 2.482 mm/s) and Fe³⁺ (*IS* = 0.424 mm/s, *QS* = 0.797 mm/s) is 45:55. The site occupancies of cations at the Fe1 and Fe2 sites given by the X-ray Rietveld analysis (*R*_{wp} = 11.84 %, *R*_c = 6.86 %, *S* = 1.73) are (Fe_{0.82}Mg_{0.18})^{Fe1}(Fe_{0.89}Al_{0.11})^{Fe2}. Unit-cell parameters are *a* 7.4656(5), *b* 12.1761(8), *c* 6.6816(4) Å, α 86.156(5)°, β 93.881(3)°, γ 112.257(4)°, *V* 560.27(6) Å³, and average Fe1-O and Fe2-O distances are 2.15 and 2.03 Å, respectively. The crystallographic features are nearly the same as those of babingtonite from other localities.

Keywords: babingtonite, Rietveld analysis, Mossbauer spectral analysis

P10.06.44*Acta Cryst.* (2008). **A64**, C503-504**Single-crystal X-ray diffraction study of chabazite at 123 K**

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