

PS08.00.14 INCOMMENSURATE PHASES OF TRIDYMITE. H.Graetsch, Institut für Mineralogie, Ruhr-Universität Bochum, D-44780 Bochum, Germany.

The third room temperature modification of tridymite, L3-T₀(MX-1), displays satellite reflections indicating an incommensurate modulation with $q \approx 2/3a^* - 1/2c^*$ (Löns, J., Hoffmann, W., Z. Kristallogr., 1987, 178, 141-143). The modulation is caused by tilting of SiO₄-tetrahedra which form rows of corner-sharing tetrahedra running parallel to the a-axis. It can be described as a combination of transverse and longitudinal displacements of the atoms without severe distortion of the tetrahedra. The modulation vector does not markedly change with increasing temperature.

Upon heating, L3-T₀(MX-1) undergoes a sequence of at least 4 phase transitions before finally transforming to hexagonal high-tridymite H1-T₀(HP) at $\approx 400^\circ\text{C}$. Three of the five high temperature modifications are incommensurate phases. At 65°C monoclinic L3-T₀(MX-1) transforms to a phase with orthorhombic metric (Hoffmann, W. et al., Fortschr. Mineral., 1983, 61, 96-98). A gap in the thermal expansion of the lattice parameters, discontinuous disappearance of the satellite reflections and a large hysteresis indicate a first order transition. The average structure of the new phase (H5-T₀) strongly resembles that of orthorhombic high tridymite H2-T₀(OC) which is known to exist between 220°C and 400°C (Dollase, W. A., Acta Cryst., 1967, 23, 617-623). However, satellites surrounding the main reflections indicate an incommensurate modulation with $q \approx 1/3a^*$. Further satellite reflections indicate an additional incommensurate modulation with a wavelength of nearly $5c_0$. At 105°C the wavelength of the modulation along the a-axis increases and several higher orders of satellite reflections appear. The already known non-integral tridymite phase H3-T₀(OS) is formed at 155°C (Nukui, A. et al., AIP Conf. Proc., 1978, 33, 327-329).

PS08.00.15 STRUCTURAL DETERMINATION OF Sr₉Ni_{6.64}O₂₁ A NEW MEMBER OF THE FAMILY A_{3n+3}A'_nB_{3+n}O_{9+6n}, (n=2). E. Gutiérrez-Puebla^a, A. Monge^a, C. Ruíz-Valero^a, I. Rasines and J. Campá^b. ^aInstituto de Ciencia de Materiales de Madrid, CSIC, Campus de Canto Blanco, E-28049 Madrid, Spain. ^bDepartamento de Cristalografía y Mineralografía. Facultad de Ciencias Geológicas. UCM. E-28040 Madrid, Spain

Within the series A_{3n+3}A'_nB_{3+n}O_{9+6n} oxides, whose structures are built up by the stacking of layers derived from perovskites, they have been recently described (1) the structure of Sr₁₂Ni_{7.5}O₂₇ is n=3 member of the series, and the structure of Ba₆Ni₅O₁₅ (2), corresponding to n=1. The aim of this work is to present the crystal structure of Sr₉Ni_{6.64}O₂₁, the n=2 member of this series.

This oxide is a new trigonal phase, related with hexagonal perovskite, having mixed [A₃O₉] and [A₃A'_nO₆] layers, where A=Sr, and A'=Ni. The Sr1 atoms are in the [Sr₃NiO₆] layer and the Sr2 is involved in the [Sr₃O₉] layer. As consequence of the less oxygen contents in the [Sr₃NiO₆] layer, the Sr1 is coordinated to eight oxygen atoms, the Sr2 atom, which is in the richest in oxygen layer, its coordination number is ten.

Ni atoms are all of them six coordinated, Ni1, Ni2 and Ni3 are octahedral but Ni4 that is the one situated in the [Sr₃NiO₆] is in the prismatic site. As consequence of the stacking sequence, octahedra sharing common opposite faces [Ni₃O₁₂] trimers and [Ni₂O₄] dimers are formed, which are connected between them through prisms, giving chains along the c direction.

1. M. Strunk und H. K. Muller-Buschbaum, *J. Alloys and Compds.* (1994), 209, 189.

2. J. A. Campá, E. Gutiérrez Puebla, M. A. Monge, I. Rasines and C. Ruíz Valero. *J. Solid State Chem.*, (1994), 108, 203

PS08.00.16 SYSTEMATIC ENUMERATION OF 3D-NETS BY COMBINING 3-CONNECTED 2D-NETS WITH 1D CHAINS. Shaoxu Han, Department of the Geophysical Sciences, the University of Chicago, Chicago, IL 60637

Systematic enumeration of 4-connected 3D nets is an important tool for solving the unknown structures of microporous materials. Many natural and synthetic framework structures have been solved by invention of new nets. Predicted structures provide a target for synthesis of phases with interesting properties.

This poster presents systematic enumeration of 3D nets based on the association of various types of simple chains with the current set of 3-connected 2D nets from the systematic databases of subunits at the University of Chicago. The algorithm in this work is to generate 3D nets by conversion of edges of 2D nets into some simple 1D chains, such as crankshaft, zigzag and saw chain. The following enumerations have been completed: (a) conversion of all edges of 2D-nets with even-numbered circuits into the 4-repeat crankshaft chain, 57 nets of which 8 occur in known structures; (b) conversion of some edges into the 2-repeat zigzag chain with the remaining edges staying horizontal, 131 nets of which 14 occur in known structures; (c) conversion of some edges into the 3-repeat saw chain with the remaining edges staying horizontal, 172 nets of which 5 occur in known structures; (d) conversion of some edges of the hex net into a crankshaft chain 80 nets selected out of the infinite number of possible ones, of which 10 occur in known structures. Some other 3D nets are also enumerated from selected 2D nets with 1D chains up to the 8-repeat pentasil chain. Each net was checked for uniqueness in the Catalog of Theoretical Frameworks using the highest space group, cell dimensions, and topological linkages as the criteria, and then the data for each new net was incorporated into the database. Furthermore, new types of nets and chains were discovered by examining models in directions parallel to the starting net.

For selected 3D nets with higher symmetry and smaller unit cell, atomic coordinates for a 3D net were derived from the model, and cell parameters and atomic coordinates were refined using distance-least-squares (DLS) program. The 3D-nets database provides a resource for search of unknown phases and this information can be used for structural determination with powder diffraction data.

PS08.00.17 MODELLING OF THE SELF-ORGANIZATION PROCESSES IN SILICATE CRYSTAL FORMING SYSTEMS. G.D. Iljushin and L.N. Demianets, Institute of Crystallography, RAS, Moscow, Russia

The model of kinetic phase transition of a disorder-order type were suggested for the crystallization in silicate-containing systems under hydrothermal conditions. The crystal-forming system from SiO₄-tetrahedra and MO_n-polyhedra (n=4 for Al, n=5 for Ti, n=6 for Zr) was chosen as a model system.

The elements of the theory of non-closed packings consisting of octahedra MO₆ and tetrahedra SiO₄ were developed (only one common apex was permitted for the connection of tetrahedron and octahedron, the number of tetrahedra was equal to the number of octahedra). The variants of the formation of MT chains and MT-layers with different topology and symmetry were found.

On the base of the theoretical ideas on the silicate formation, the algorithm of matrix assembling of the known crystal structures of zirconosilicates, titanosilicates and aluminosilicates was determined. The analysis of the symmetry data for silicates was carried out using the author's method of crystal structural intersections of space groups of symmetry. This method provides a possibility to identify the channels of structure evolution depending on growth conditions. In the framework of the model, the mechanism of the Si-radical formation from isolated SiO₄-tetrahedra (chains, rings, layers, framework) is described.