INORGANIC AND MINERAL COMPOUNDS

PS08.00.14 INCOMMENSURATE PHASES OF TRIDYMITE. H. Gnesch, Inst. f. Mineralogie, Ruhr-Universitats Bochum, D-44780 Bochum, Germany.

The third room temperature modification of tridymite, L3-T3 (MX-1), displays satellite reflections indicating an incommensurate modulation with q = 2j/a1<1/2j (Lons, 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-T3 (MX-1) undergoes a sequence of at least 4 phase transitions before finally transforming to a hexagonal high-tridymite H1-T3 (EP) at ~400°C. Three of the five high temperature modulations are incommensurate phases. At 65°C monoclinic L3-T3 (MX-1) transforms to a phase with orthorhombic orthoboric (Hoffmann, W. et al., Fortschr. Mineral., 1983, 61, 36-58). 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 (E11-T3) strongly resembles that of orthorhombic high tridymite H2-T3 (OC) which is known to exist between 220°C and 400°C (Dollase, W.A., Acta Cryst., 1967, 33, 617-623).

However, satellites surrounding the main reflections indicate an incommensurate modulation with q = 1/3a1. Further satellite reflections indicate an additional incommensurate modulation with a wavelength of nearly 5c1. 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 H5-T0 (Gutierrez-Puebla, I., Rasines and J. Campa, I. Instituto de Ciencia de Materiales de Madrid, CSIC, Campus de Canto Blanco, E-28049 Madrid, Spain; Departamento de Cristalogr. y Minera~rografia, Facultad de Ciencias Geologicas, UCM, E-28040 Madrid, Spain)

Within the series A3n+3AnB3+n09+6n oxides, whose structures are built up by the stacking of layers derived from perovskites, they have been recently described (1) the structure of Sr3Ni6.64021 A. Gutierrez-Puebla, A. Monge, C. Ruiz-Valero, I. Rasines and J. Campa, I. Instituto de Ciencia de Materiales de Madrid, CSIC, Campus de Canto Blanco, E-28049 Madrid, Spain; Departamento de Cristalogr. y Mineralografia, Facultad de Ciencias Geologicas, UCM, E-28040 Madrid, Spain

PS08.00.15 STRUCTURAL DETERMINATION OF Sr9Ni6.64021 A NEW MEMBER OF THE FAMILY A3n+3AnB3+n09+6n (n=2). E. Gutierrez-Puebla, A. Monge, C. Ruiz-Valero, I. Rasines and J. Campa, I. Instituto de Ciencia de Materiales de Madrid, CSIC, Campus de Canto Blanco, E-28049 Madrid, Spain; Departamento de Cristalogr. y Mineralografia, Facultad de Ciencias Geologicas, UCM, E-28040 Madrid, Spain

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 Mn0-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.