

**05.1-38** ON THE ORTHO-CLINO PHASE TRANSITION OF FERROSILITE ( $\text{FeSiO}_3$ ) AND Fe-RICH PYROXENES.

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Temperature induced orthorhombic ( $Pbca$ )-monoclinic ( $C2/c$ ) pyroxene phase transition was studied using high-temperature precession camera method. The starting materials were synthetic ortho-pyroxenes with the composition of (Fs), ( $\text{Wo}_{.02}\text{Fs}_{.98}$ ), ( $\text{Wo}_{.05}\text{Fs}_{.95}$ ), [ $\text{Wo}_{.05}(\text{Fs}_{.75}\text{En}_{.25})_{.95}$ ], ( $\text{Fs}_{.9}\text{En}_{.1}$ ) and ( $\text{Fs}_{.8}\text{En}_{.2}$ ) where  $\text{Fs}=\text{FeSiO}_3$ ,  $\text{Wo}=\text{CaSiO}_3$  and  $\text{En}=\text{MgSiO}_3$ . Ortho-pyroxene with the Fs composition showed reversible and topotaxial transformation to the twined clino-pyroxene at  $1020^\circ\text{C}$  with the orientation ( $a_{\text{ortho}}/a_{\text{clino}}$ ,  $c_{\text{ortho}}/c_{\text{clino}}$ ). Wo free pyroxenes transformed to clino-phase topotaxially with the orientation same as those on Fs, but they did not transform reversibly to the ortho-phase on cooling. The pyroxenes with Wo composition transformed rapidly to twined clino-phase but the orientations between both phases were quite haphazard for each run.

Smyth has suggested that on the coherent pyroxene transition M1 site in ortho-phase becomes M2 site in clino-phase and M2 site in ortho-phase becomes M1 site in clino-phase (Smyth, Amer. Mineral. (1974) 59, 345). The results of the present study may support his suggestion as the coherent pyroxene transitions were observed only on pure Mg and Fe end-member pyroxenes in which both M-sites are occupied only by Mg and Fe. In ortho-pyroxene, Ca ion is in M2 site and it could not be entered to M1 site in clino-phase because of its large ionic radius. This makes the coherent transition impossible and brings about the "nucleus and growth type" transition. Whereas smaller Mg ion is in M1 site in ortho-phase and it may be allowed to enter M2 site in clino-phase, but may result in some distortion in clino-phase structure which prevents the reverse transition to ortho-pyroxene on the cooling stage.

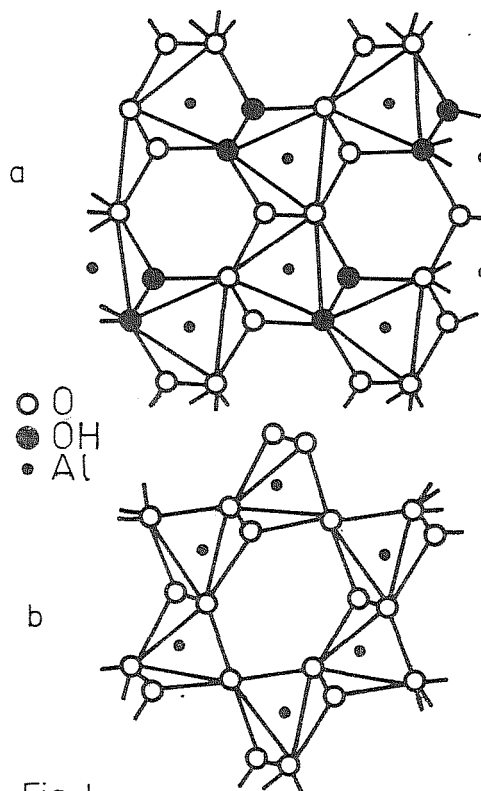


Fig. 1

**05.1-39** THERMAL BEHAVIOUR OF MUSCOVITE - OD STRUCTURAL ASPECTS. By K. Dornberger-Schiff and K.-O. Backhaus, Central Institute of Physical Chemistry, Academy of Sciences of the G.D.R., Berlin-Adlershof, German Democratic Republic

Muscovite crystals are known to undergo irreversible changes when heated. These changes differ qualitatively when heated up to temperatures  $T < 700^\circ$  and  $T > 700^\circ$ .

In order to elucidate the changes in structure, Weissenberg diagrams of heat-treated muscovite single crystals  $2M_1$ , quenched after heating, have been taken and discussed: higher temperature treated (HTT) and lower temperature treated (LTT) compared with  $700^\circ$ . ( $hkl$ ) reflections (orthohexagonal) with  $k \neq 3n$  are diffuse (direction  $c^*$ ) for LTT and HTT crystals, ( $hkl$ ) with  $k=3n$  are different from the untreated crystals only for the HTT crystals.

Furthermore, IR investigations showed that no H atoms are present in the HTT crystals, indicating the loss of every second OH group together with the H atom of the other OH group, in agreement with earlier results (Peucker, private communication). The results of structure determinations of LTT and/or HTT crystals, carried out also with the help of OD theory, are to be presented.

Fig. 1 Tentative structure of a) octahedral (idealized) sheet before, b) after dehydroxylation (5-coordinated).

**05.1-40** RIGID-BODY ANALYSIS OF DIAMANTANE AT 7 K.

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Diamantane ( $\text{C}_{14}\text{H}_{20}$ ) is a cage-like molecule which at room temperature crystallises in  $Pa3$ . It has been shown by Raman spectroscopy (Jenkins and Bates, J. Phys. C: Solid State Physics (1979) 12, 1003) that a phase transition occurs at 35 K involving a change of space group. Neutron Bragg intensities have been collected at 7 K, and the results of a rigid-body analysis of these will be presented. Preliminary results indicate no change of space group and no substantial reorientation about the three-fold axis.