THE EFFECT OF CLASS 1 H_2O ON A RAMAN ACTIVE T_2 STRETCHING MODE IN Mg-CORDIERITE

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The structure of orthorhombic cordierite consists of six-membered (Al, Si)O_4 rings, which are laterally linked by additional (Al, Si)O_4 tetrahedra. Stacked rings form channels parallel *c* which can incorporate volatiles like H_2O and CO_2 in various amounts. Octahedral sites contain mainly Mg and Fe. Five tetrahedrally coordinated sites and channel sites have to be distinguished in the structure: $(M)_2(T_11)_2(T_26)_2(T_23)_2(T_21)_2(T_16)O_{18}$(Ch0,Ch1/4) (e.g. BERTOLDI et al., 2004). In orthorhombic cordierite Si and Al are fully ordered. The ring tetrahedra T_21 and T_23 contain Si and T_26 contains Al. H_2O is incorporated into the Ch1/4 positions and two classes of H_2O can be distinguished: class 1 H_2O, which is subdivided in three types with different orientations and class 2 H_2O, which interacts with alkali cations and is subdivided in two types with different orientations (KOLESOV & GEIGER, 2000).

Raman spectroscopic investigations of alkali-free synthetic Mg-cordierites with H_2O contents of 0 – 2 wt.% revealed a guest-host interaction between class 1 H_2O and Si-channel tetrahedra. A peak at 1189 cm^{-1} in anhydrous Mg-cordierite is assigned to T_21 and T_23 stretching vibrations (KAINDL et al., 2011). The peak shifts towards lower energies with increasing H_2O contents and occurs at 1186 cm^{-1} in samples with 2 wt.% H_2O. The channel volatiles (H_2O, CO_2) of natural Mg-rich cordierite (from White Well, Australia) were removed by heating. The comparison of the Raman spectra before and after heating yields a 4 cm^{-1} peak shift at 1189 cm^{-1} towards higher energies. An arrestive effect of H_2O and other channel volatiles to the symmetric vibration of adjacent $T_{2(Si)}$ tetrahedra can be described with Raman spectroscopy.

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