Raman spectroscopic investigation of Al-bearing orthopyroxene

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Raman mode shift reflects the chemical composition change of solid-solution series. Early study showed that red-shifts in Raman modes observed in pyroxenes presenting strong correlation of Mg-Fe-Ca substitution in M-octahedral sites [1]. Aluminum is also another element found in natural pyroxene. The incorporation of Al³⁺ in pyroxene will affect not only the elasticity but also enhance the coupling of [H⁺] into structure. Different from Mg²⁺, Fe²⁺ and Ca²⁺ occupying M sites, the Al³⁺ ion has been shown to be occupied T and M sites [2].

In order to investigate the Raman shift as function of Al-content, we synthesized a series of Al-bearing OEn crystals, up to 18 Al₂O₃ wt% at different pressure and temperature. Polarized Raman spectra of Al-bearing OEn crystals were collected parallel and normal to the crystallographic axis c at ambient conditions. We observed some Raman modes for this suite of Al-bearing OEn presented obvious blue shift above 600 cm⁻¹. The Raman mode shift of the pairs of 660/680 and 1010/1030 cm⁻¹ do not show strong positive correlation as Al³⁺-content increasing and presents a red shift when Al₂O₃ increases more than 10 wt%. Single-crystal X ray diffraction results of Al-OEn showed that the cell volume decreases as the Al-content increases and the behavior of Al partitioning in M and T sites changed around 4-5 Al₂O₃ wt%. Atomic simulation was performed to understand the relation between the crystal structure and Raman mode vibrations. We will present the results and analysis in the meeting.