

Raman scattering of omphacite at high pressure: Toward its possible application to elastic geothermobarometry

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ABSTRACT

Due to their widespread occurrence in several geological settings, omphacite inclusions could be used for elastic Raman geothermobarometry. However, the Raman scattering of complex silicate minerals entrapped in a host depends on both the chemical composition and elastic strain developed during the metamorphic pathway, which makes the task very challenging. Here, as a very first step to probe the potential of omphacite to be used as a mineral inclusion in elastic geothermobarometry, we report the pressure dependence of the Raman spectra of omphacite crystals with the same composition, approximately $\text{Jd}_{43}\text{Di}_{57}$, but having different symmetry because of the existence ($P2/n$) or absence ($C2/c$) of chemical order at the six- and eight-coordinated cation sites. The experimental results are complemented by ab initio quantum mechanical simulations on fully ordered omphacite ($\text{Jd}_{50}\text{Di}_{50}$). We demonstrate that the position of the well-resolved Raman peak near 688 cm^{-1} , arising from Si-O-Si bond bending, is very sensitive to pressure but independent of the state of chemical order, which makes it promising to be utilized in Raman geobarometry. The width of this peak varies with chemical order but not with pressure and therefore can be used to constrain the temperature of inclusion entrapment, because the chemical order is indicative of the closure temperature of the cation-exchange reaction. However, further detailed analyses on the compositional variation of the Raman spectra of omphacite is required before considering omphacite-in-garnet systems to be suitable for Raman elastic geothermobarometry.

Keywords: Omphacite, site-occupancy order, Raman spectroscopy, high pressure, ab initio calculation