[1], allowed us to measure sound wave velocities at pressures up to about 7 GPa and temperatures up to 873K. Results from both the ultrasonic measurements and Xray diffraction will be presented as well as the effect of Fe content on the elastic properties of olivine. Finally, the implications for the determination of a mineralogical model in the context of the Mars Insight SEIS experiment will be discussed.

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Elastic geobarometry using omphacite in eclogites: a Raman spectroscopy approach

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Raman scattering is very sensitive to structural deformations in crystal structures developed upon heating or compression. Raman elastic geobarometry uses deformation recorded by a mineral inclusion trapped in its host to retrieve the pressure and temperature conditions at which the inclusion has been entrapped [1]. Several host-inclusion systems have been studied, but clinopyroxenes have not yet been investigated. Because of their widespread occurrence in several geological settings and rock-types (e.g. high pressure eclogites, mantle xenoliths etc.), omphacitic clinopyroxenes (solid solution of jadeite, augite and aegirine, with chemical formula (Ca,Na)(Mg,Al)Si_2O_6) should be exploited for application of elastic geothermobarometry. However, he application of this methodology to omphacites requires the accurate knowledge of their elastic behaviour and at least a detailed Raman spectroscopy calibration as a function of external compression.

For this purpose, we have studied ordered and disordered omphacite crystals (belonging to Münchberg Massif, Bavaria, Germany [2]) by in situ high-pressure Raman spectroscopy and the results have been compared against calculated Raman spectra obtained by performing ab initio simulations on a completely ordered omphacite. Ab initio simulations have been carried out at variable pressures by means of ab initio hybrid HF (Hartree-Fock)/DFT (Density functional theory) simulations using the CRYSTAL17 software [3] following the protocol developed by [4]. The calculations resulted to be in good agreement with the experimental data. The full set of 60 Raman active modes and their intensities have been calculated at variable pressures and the main Raman peaks have been assigned to specific atomic motions.

Our results readily enabled us to calculate the entrapment pressure of omphacite inclusions still trapped in their host rocks by determining the changes in the Raman shift of the main peaks.

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