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Structure determination of CaSiO3 wollastonite polymorphs at HP/HT conditions by single crystal in-situ diffraction

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CaSiO3 wollastonite and its polymorphs are very interesting since they represent the major pure calcium silicate in different geological settings. In the upper-crust, wollastonite and its common polytype parawollastonite (wollastonite 2M) are stable in specific metamorphic reaction zones (skarns), while the high-temperature ambient pressure polymorph pseudowollastonite is associated to Ca-rich paralavas and hornfels. At pressure above 3 GPa, the breyite-structured polymorph, stable over a wide range of temperatures and pressures, has been found in diamonds as one of the most abundant inclusions [1].
The structural evolution with pressure of wollastonite and breyite is characterized by several phase transitions to denser structures [2]. We report new data on high pressure structural and elastic properties on wollastonite 2M and pseudowollastonite, based on in-situ single crystal diffraction experiments at high-pressure and high-pressure/high-temperature conditions.
We used resistively heated Diamond Anvil Cell at XPRESS beamline (Elettra, Trieste). We performed multiple single crystal diffraction, exploiting the relatively large beam available at the beamline. In this way we have been able to collect simultaneously two sample crystals with different crystallographic orientation and two reference crystals, suitable both for increasing reciprocal space coverage for low symmetry samples, and for P and T determination, together witth spectroscopic methods and direct temperature measurements by thermocouples.
The wollastonite 2M polymorph showed a phase transition to a triclinic structure above 8.5 GPa, while for the pseudowollastonite no phase transition was observed in the pressure range from 0 to 16 GPa, in contrast with previous literature data [3]. The HP/HT data confirm the stability of the triclinic wollastonite polymorph at upper mantle conditions, and allow the determination of thermal equation of state parameters. The identification of stable and metastable high-pressure polymorphs could be extremely useful also to interpret shock wave experiments on these systems [4].

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