

# Structure and equation of state of Ti-bearing davemaoite: new insights into the chemical heterogeneity in the lower mantle

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Davemaoite, or  $\text{CaSiO}_3$  perovskite, is considered the third most abundant phase in the pyrolytic lower mantle and the second most abundant phase in the subducted mid-ocean ridge basalt (MORB). During the partial melting of the pyrolytic upper mantle, incompatible titanium (Ti) becomes enriched in the basaltic magma, leading to the formation of Ti-rich MORB. Davemaoite is considered an important Ti-bearing mineral in subducted slabs by forming a solid solution known as  $\text{Ca}(\text{Si},\text{Ti})\text{O}_3$ . However, the crystal structure and elastic properties of  $\text{Ca}(\text{Si},\text{Ti})\text{O}_3$  perovskite solid solution at relevant pressure and temperature conditions have not been systematically investigated. In this study, we studied the structure and equations of state of  $\text{Ca}(\text{Si}_{0.83}\text{Ti}_{0.17})\text{O}_3$  and  $\text{Ca}(\text{Si}_{0.75}\text{Ti}_{0.25})\text{O}_3$  perovskites at room temperature up to 82 GPa and 64 GPa, respectively, by synchrotron X-ray diffraction (XRD). Both  $\text{Ca}(\text{Si}_{0.83}\text{Ti}_{0.17})\text{O}_3$  and  $\text{Ca}(\text{Si}_{0.75}\text{Ti}_{0.25})\text{O}_3$  perovskites were found to adopt a tetragonal structure up to the maximum pressures investigated. Comparing the results from this study with pure  $\text{CaSiO}_3$  davemaoite, we determined that both Ti-bearing davemaoite are expected to be less dense up to the core-mantle boundary (CMB), and specifically ~1-2 % less dense than  $\text{CaSiO}_3$  davemaoite in the pressure range of the transition zone (15-25 GPa). Our results indicate that the presence of Ti-bearing davemaoite phases could potentially lead to a reduction in the average density of the subducting slabs, which in turn promotes the stagnation of subducted slabs in the upper lower mantle. Furthermore, the presence of low-density Ti-bearing davemaoite phases and subduction of MORB in the lower mantle could provide an explanation for the seismic heterogeneity in the lower mantle, including the presence of the large low shear velocity provinces (LLSVPs) in the lowermost mantle.