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Structural refinements of magnesite at very high pressure

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ABSTRACT

Unit-cell parameters of magnesite were measured between ambient pressure and 80 GPa using angle dispersive powder X-ray diffraction. The isothermal bulk modulus determined from a third order Birch Murnaghan equation of state is $K_T = 108(3)$ GPa with $K'_T = 5.0(2)$, and $V_0 = 279.2(2)$ Å^3, in agreement with previously reported values. Combining this result with previous measurements, we show that magnesite with $R\bar{3}c$ structure is stable compared to the assemblage periclase + carbon dioxide at pressures and temperatures corresponding to the core-mantle boundary. Crystal structure refinements have also been carried out up to 80 GPa. The main structural change is a strong compression of the MgO_6 octahedra with increasing pressure, largely reflected in the anisotropic compression of the **c** axis. This compression, however, tends to level off at around 50–60 GPa. On the other hand, the CO_3 groups do not remain invariant since they undergo first a slight expansion and then a compression above the same threshold pressure of 60 GPa above which Mg-O bonds cannot compress further. Thus, in this structure-type, the energy gain due to a drastic volume reduction of the MgO_6 octahedron compensates in a given pressure range for the energy cost of the small expansion of the CO_3 carbonate unit.