Stabilities of $MgCO_3$ polymorphs up to 150 GPa

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The possible coexistence of silicates and $MgCO_3$ was proposed for cold and oxidized oceanic slabs in the lowermost mantle [1]. Above 80 GPa and 2000 K, model predictions and X-ray powder diffraction experiments have indicated that $MgCO_3$ (magnesite) transforms into a new polymorph $MgCO_3$-II with space group C2/m, where carbon becomes tetrahedrally coordinated by oxygen and forms $\{C_3O_9\}^{6-}$ rings with sp^3 hybridized bonds [1,2]. However, alternative structures have also been proposed for the same P,T-conditions [3].

Here, we report the phase relations in $MgCO_3$ as observed by Raman spectroscopy at high pressures (≤148 GPa) after applying high temperatures (≤3600 K) in CO_2 laser-heated diamond anvil cell experiments (LH-DAC). Our study provides the first Raman spectra of pure $MgCO_3$ at pressures >55 GPa. Synchrotron X-ray powder diffraction data were obtained at a pressure of 110 GPa. Density functional theory-based model calculations were used to compute Raman spectra for several $MgCO_3$ high pressure polymorphs. By combining the experimental observations with the DFT-results, we constrain the phase stability field of $MgCO_3$ with respect to the high pressure polymorph, $MgCO_3$-II.

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[1] Maeda et al. (2017), *Sci. Rep.* **7**, 40602. [2] Oganov et al. (2008), *EPSL* **273**, 38-47. [3] Pickard & Needs (2015), *Phys. Rev.* B **91**, 104101.