Poster Presentation

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Transformation pathways of structural transitions between BaMg(CO3)2 polymorphs

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In-situ investigations on BaMg(CO3)2 (= α-phase, space group R-3c) by means of single-crystal diffraction and Raman spectroscopy yield the existence of novel structural polymorphs at high-pressure (γ-phase, C2/c) and high-temperature (β-phase, R-3m) conditions. Isothermal hydrostatic compression at room temperature yield a high-pressure phase transition at Pc ≈ 2.32 ± 0.04 GPa, which is weakly first order in character and reveals significant elastic softening of the high-pressure form (α: K0 = 66.2 ± 2.3 GPa, dK/dP = 2.0 ± 1.8; γ: K0 = 41.9 ± 0.4 GPa, dK/dP = 6.1 ± 0.3). X-ray structure determination confirms a distorted but topologically similar crystal structure of the γ-phase, with Ba in twelve-fold and Mg in octahedral coordination together with characteristic CO3 units. Based on the experimental series of in-situ HPHT data points, the phase boundary of the α-to-γ-transition was determined with a Clausius-Clapeyron slope of 9.8(7) × 10-3 GPa K-1. In-situ measurements of the X-ray intensities carried out to identify the nature of the structural variation correspond to the previously reported transformation from α- to β-BaMg(CO3)2 at 343 K and 1 bar. The investigations revealed, in contrast to all X-ray diffraction data recorded at 298 K, the disappearance of the superstructure reflections and the observed reflection conditions confirm the anticipated R-3m space-group symmetry. The pathway of structural transformation follows a typically displacive fashion, involving exclusively positional shifts of the oxygen atoms for the α-β-transformation. In contrast, in the atomic displacement of the Ba atoms in addition to the three crystallographically independent oxygen sites is responsible for a comparably higher flexibility of the C2/c structure, which explains the origin of the remarkable elastic softening.

Keywords: phase transition, high-pressure structure, carbonate