

High-pressure compressibility and vibrational properties of (Ca,Mn)CO₃

JIN LIU^{1,*}, RAZVAN CARACAS², DAWEI FAN³, EMA BOBOCIOIU², DONGZHOU ZHANG⁴, AND
WENDY L. MAO^{1,5}

¹Department of Geological Sciences, Stanford University, Stanford, California 94305, U.S.A.

²CNRS, Laboratoire de Géologie de Lyon, Université Claude Bernard Lyon 1, 69342 Lyon Cedex 07, France

³Key Laboratory of High-temperature and High-pressure Study of the Earth's Interior, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang, Guizhou 550002, China

⁴Hawai'i Institute of Geophysics and Planetology, University of Hawai'i at Manoa, Honolulu, Hawaii 96822, U.S.A.

⁵Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, California 94025, U.S.A.

ABSTRACT

Knowledge of potential carbon carriers such as carbonates is critical for our understanding of the deep-carbon cycle and related geological processes within the planet. Here we investigated the high-pressure behavior of (Ca,Mn)CO₃ up to 75 GPa by synchrotron single-crystal X-ray diffraction, laser Raman spectroscopy, and theoretical calculations. MnCO₃-rich carbonate underwent a structural phase transition from the CaCO₃-I structure into the CaCO₃-VI structure at 45–48 GPa, while CaCO₃-rich carbonate transformed into CaCO₃-III and CaCO₃-VI at approximately 2 and 15 GPa, respectively. The equation of state and vibrational properties of MnCO₃-rich and CaCO₃-rich carbonates changed dramatically across the phase transition. The CaCO₃-VI-structured CaCO₃-rich and MnCO₃-rich carbonates were stable at room temperature up to at least 53 and 75 GPa, respectively. The addition of smaller cations (e.g., Mn²⁺, Mg²⁺, and Fe²⁺) can enlarge the stability field of the CaCO₃-I phase as well as increase the pressure of the structural transition into the CaCO₃-VI phase.

Keywords: Carbonate, X-ray diffraction, raman spectroscopy, high pressure