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# High Pressure Structural Studies on BaCO<sub>3</sub> up to 20 GPa

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## BACKGROUND

Carbonate compounds are thought to make up a minor portion of the Earth's upper mantle. Shock heating of the surfaces of carbonate rocks, as in the instance of a meteor impact, has the potential to affect CO<sub>2</sub> concentrations in the Earth's atmosphere. The bulk-modulus of carbonate materials is directly proportional to the rate of devolatilization under these conditions [1]. The interest in Barium Carbonate (BaCO<sub>3</sub>) specifically is motivated by its structural proximity to aragonite carbonates. Crystalline phase transitions occur in aragonite under extreme conditions that are difficult to maintain in a laboratory; BaCO<sub>3</sub> is isostructural with aragonite and therefore is expected to have similar phase transitions at conditions easier to simulate in a laboratory. Studies of Barium carbonate will not only lead to conclusions about witherite carbonates, but aragonite carbonates as well [1]. Another, use of Barium carbonate is in ceramic glazes [4]. Under extreme conditions (firing in a kiln) the structural transition of BaCO<sub>3</sub> provides changes necessary for interesting glazes. This experiment was conducted with an aim of understanding the phase transition behavior of BaCO<sub>3</sub> under pressure and providing more detailed analysis of the high pressure phase by extending the pressure range previously investigated [1,2,3].

## EXPERIMENTAL

The crystal structure of witherite BaCO<sub>3</sub> was studied using powder X-Ray diffraction through a Merrill-Bassett diamond anvil cell to high pressures up to 20 GPa. The powder form was loaded with ruby in a Re gasket with a 150 μm hole and 4:1 methanol-ethanol pressure medium. X-rays used for the experiment were of incident wavelength 0.36793 Å and were generated by the synchrotron at Argonne National Laboratory at the ID-B station in sector 16. The pressure was measured at room temperature using an offline ruby system and was increased in intervals of approximately 2 GPa. XRD patterns were taken for an exposure time of 15-30 seconds. The patterns were integrated using Fit2D. The structural analysis was performed using JADE and EOS Fit.

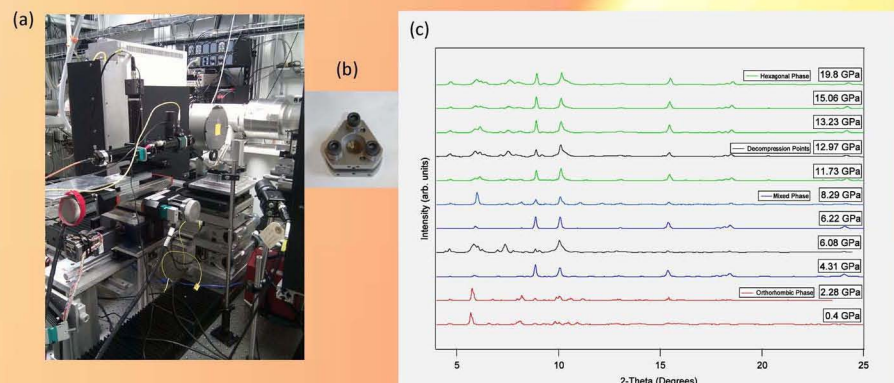


Fig.1 (a) High pressure x-ray diffraction set up at ID-B station at HPCAT, Argonne National Laboratory (b). Merrill-Bassett type high pressure diamond anvil cell. (c). Representative x-ray diffraction patterns at various pressures up to 19.8 GPa for BaCO<sub>3</sub>.

## RESULTS

BaCO<sub>3</sub> crystallizes in the orthorhombic structure with space group *Pmcn* and the lattice parameters are found to be *a* = 5.3017 Å, *b* = 8.90274 Å, and *c* = 6.42761 Å. These parameters compare well with literature [1,2]. Between 4 and 8 GPa a pressure induced first-order phase transition is observed to a hexagonal structure with space group *P-31c*. During this interval, a mixed phase is observed. After the phase transition, an axial anisotropic compressibility (as the *b* axis intersects with the *a* axis) is observed in our experiments. The variations of *d*-spacings as a function of pressure are shown in figure 2(a). From the cell parameter values found in JADE, the volume has been obtained for each pressure and is shown in figure 2(b) where the orthorhombic, mixed, and hexagonal phases are plotted. A third-order Birch-Murnaghan equation was used to fit the high-pressure phase of our P-V data.

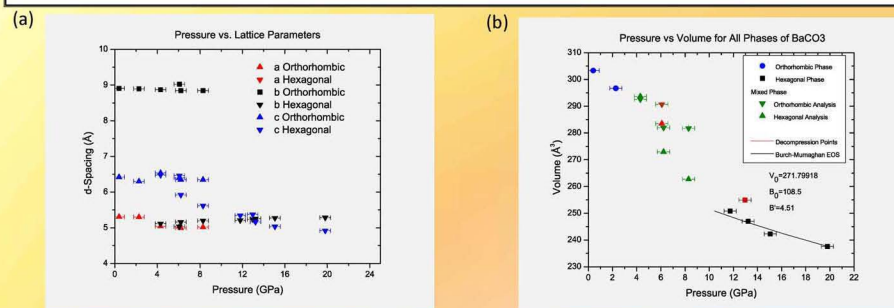


Fig.2 (a). Variation of lattice parameters of BaCO<sub>3</sub> phase as a function of pressure (b). P-V plot of all phases

## CONCLUSIONS AND SUMMARY

The orthorhombic structure is stable up to 4.3 GPa. At 4.3 GPa diffraction peaks representing the hexagonal phase begin to appear compared to the previously found exposure range of approximately 8 GPa [1,2,3]. In our experiment, diffraction peaks from both the orthorhombic structure and the hexagonal structure co-exist until after 8 GPa. After 8 GPa, a complete phase transformation to the hexagonal phase with space group *P-31c* was observed. The phase change represented in the P-V data does not reflect a steep change in volume as pressure increases as found previously [1].

## REFERENCES

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