Phase transition of strontium carbonate

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Introduction

The geochemistry of carbon at depth within the planet is complex: depending on pressure, temperature and oxygen fugacity, carbon may occur in its elemental form (either as graphite or diamond), as carbonate groups present in either minerals or magmas, or in a carbon-rich fluid. Extensive experimental work has been conducted to understand the conditions under which diamonds may be synthesized to examine the phase equilibria of carbon in silicate assemblages at high pressures, and to explore the pressure-induced phase transitions of carbonates. However, there have been relatively few *in situ* studies of the stability and structure of carbonates under pressures and temperatures corresponding even to those of the shallow upper mantle.

Experimental methods

High-pressure X-ray diffraction experiments were performed using a laser-heated diamond anvil cell (LHDAC) high-pressure apparatus. Synthetic powdered SrCO₃, (purity 99.99%) was loaded into a 50-100 µm diameter hole that was drilled into a rhenium gasket using an excimer laser. Platinum powder was mixed with the sample to absorb the laser radiation to provide a heat source, and was also used as an internal pressure calibrant. NaCl was used as a pressure transmitting medium to reduce deviatric stress and temperature gradients in the sample. The samples were heated with either a YAG laser to overcome any potential kinetic effects on possible phase transitions. The pressure was determined from the observed unit cell volume of platinum using the Pt equation of state. The samples were probed using an angle-dispersive X-ray diffraction technique at the synchrotron beam lines BL13A, Photon Factory in Japan [1]. A monochromatic incident X-ray beam with a wavelength of about 0.42 angstrom was used. The X-ray beams were collimated to a diameter of 50 µm, and the angle-dispersive X-ray diffraction patterns were obtained on an imaging plate (Rigaku).

Results and Discussion

In the first set of experiments, the pressure was increased directly to 10 GPa at room temperature, and an X-ray diffraction pattern of the sample was recorded. The diffraction pattern of the sample showed the aragonite structure. This indicated that no phase transition had occurred during the compression. However, a strainbroadening of the diffraction peaks occurred, resulting from the large differential stress that was induced in the diamond anvil cell experiments as pressure increased. After the desired pressure was achieved, the sample was heated to about 1500 K to relax the differential stress and to overcome potential kinetic effects on possible phase transitions. After heating, the pressure had decreased to 8.2 GPa, and the diffraction peaks became sharp because of the release of differential stress. However, no new peaks appeared in the diffraction pattern (Fig. 1). In the next set of experiments, the pressure was increased directly to about 15 GPa, and the sample was then heated. After the heating at 14.5 GPa, some new peaks appeared in the diffraction pattern. This indicates that the starting material had transformed to a new high-pressure, postaragonite phase, shown in Fig. 1. The post-aragonite phase was unquenchable: when the pressure was reduced to ambient conditions, the sample transformed into the two orthorhombic phases (Fig. 1). Further runs were performed to 32 GPa. The transition pressure from the aragonite-type to the post-aragonite phase is located at about 10 GPa. The crystal structure of the post-aragonite phase of SrCO₃ is likely to have an orthorhombic symmetry. The number of molecules of this phase in a unit cell (Z) is 2.

References

[1] Ono et al., Phys. Earth Planet. Inter. 131, 311 (2002).

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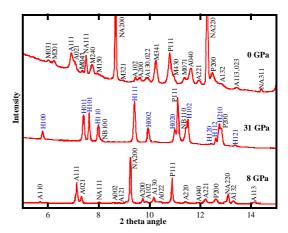


Figure 1.

Observed X-ray diffraction patterns of the samples at 300 K. Top, aragonite and metastable orthorhombic phase at 0 GPa after decompression; middle, post-aragonite type at 31 GPa; bottom, aragonite-type at 8 GPa. Abbreviations of peaks are as follows: M, metastable orthorhombic phase; A, aragonite; H, post-aragonite; P, platinum; NA, B1-type sodium chloride; NB, B2-type sodium chloride.