

Pressure induced amorphization of portlandite, $\text{Ca}(\text{OH})_2$ around 6 GPa

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Introduction

Portlandite, $\text{Ca}(\text{OH})_2$, has a basic layer type structure. There are hydrogen bonds in the interlayer. Its structure is important to understand the behavior of hydrogen bonding with variations of pressure and temperature. According to previous study using powder X-ray diffraction methods, portlandite translated to an amorphous state around 11 GPa at ambient temperature^[1],^[2]. Moreover, another spectroscopic studies showed higher transition pressure (16.6 GPa)^[3]. In this way, the transition pressures of previous studies were significantly different by experimental conditions (*ex.* pressure medium and methods). The hydrostatic situation would influence in this phenomena.

In this study, therefore, to investigate the transition pressure of portlandite, single crystal X-ray diffraction method were conducted using the 4:1 fluid mixture of methanol and ethanol, which can keep higher hydrostatic conditions up to 10 GPa, as pressure medium.

Experimental Procedure

The sample used for this study was synthesized by the chemical reaction: $2\text{NaOH}_{\text{aq}} + \text{CaCl}_2 \rightarrow \text{Ca}(\text{OH})_2\downarrow + 2\text{NaCl}$. A single crystal of portlandite ($50 \times 50 \times 50 \mu\text{m}^3$ in size) was mounted in a modified Merrill-Bassett type diamond anvil cell with a small piece of a ruby crystal, which used for the pressure calibration. The 4:1 fluid mixture of methanol and ethanol was used for the pressure medium and a SUS301 stainless plate used for a gasket. Pressure was determined by the ruby fluorescence method [4]. The wavelength of X-ray radiation was calibrated by the unit cell volume of the ruby standard crystal at ambient temperature ($\lambda = 0.7 \text{ \AA}$).

The X-ray diffraction intensities were measured using an automated four-circle X-ray diffractometer installed at the beam line BL-10A, Photon Factory, High Energy Accelerator Research Organization. To check the phase transition to amorphous state for portlandite, oscillation photographs were taken at some pressure points (5.5, 8.3 GPa and 3.0 GPa [reducing process]). Each exposing time is about 30 minutes.

Results

Portlandite structure were kept at least up to 5.5 GPa. Figure 1 showed the diffraction spots, which were indexed, from portlandite structure at 5.5 GPa. Other spots were from diamond anvils and rings were from Be backing plates. Over this pressure, portlandite translated to an amorphous state at 8.3 GPa (Figure 2). The spots

such as {001} and {011}, which were observed at 5.5 GPa, disappeared or observed very weak around this pressure. After reducing pressure to 3.0 GPa, the peaks recovered but the forms of spots changed to broad one (Figure 3). These results show that this transition is reversible and would be displace type.

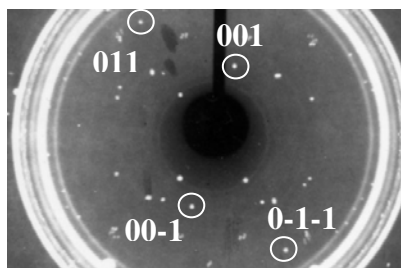


Figure 1. Oscillation photograph of portlandite at 5.5 GPa (Before transition).

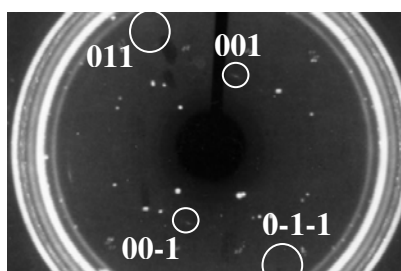


Figure 2. Oscillation photograph of portlandite at 8.3 GPa (After transition).

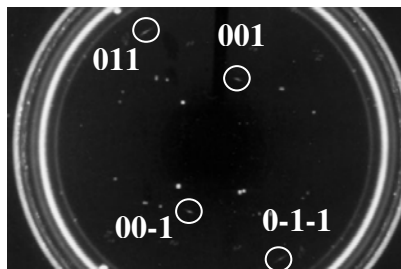


Figure 3. Oscillation photograph of portlandite at 3.0 GPa (After reducing pressure).

References

- [1] Meade *et al.* (1990), *Geophys. Res. Lett.*, **17**, 1157-1160
- [2] Nagai *et al.* (2000) *Phys. Chem. Miner.*, **27**, 462-466
- [3] Ekbundit *et al.* (1996), *J. Solid State Chem.*, **126**, 300-307
- [4] Piermarini *et al.* (1975) *J. Appli. Phys.*, **46**, 2774-2780

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