

Structural Study of Approximant Crystal of Cd-Yb Quasicrystal Under High Pressure and High Temperature

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Very recently, Tsai et al. found binary quasicrystals in Cd-M (M=Yb, Ca) alloy system, which is a first example of a two-component stable icosahedral quasicrystal [1]. This system has additional characteristic feature, that is the existence of approximant crystal whose chemical composition is very close to the quasicrystals; Cd 85.1: Yb 14.9 for quasicrystal phase, and Cd 85.7: Yb 14.3 (Cd₆Yb₁) for cubic 1/1 approximant crystal phase. The structure is similar to each other in local region [2]. And, our previous work shows that the crystal structure of the approximant crystal phase is not stable under pressure while the quasicrystal phase is stable, which is derived from steep diffraction line broadening of the approximant phase even in low pressure region. So, we consider it is probable that the crystal phase transforms to the quasicrystal phase under high pressure and high temperature. So, we performed powder X-ray diffraction measurements of Cd-Yb approximant crystal phase under high pressure and high temperature at BL10XU.

High pressure and high temperature condition was generated with use of a conventional DAC and a ring heater set around anvils. The heater was made from Pt-Rh wire, and was sustained by mica sheets in order to avoid direct contact to the anvil cell.

Sample temperature was monitored by a thermocouple (K) of 0.1 mm in diameter which was in contact with one of the anvils. High pressure argon gas was sealed in the DAC with the sample as a pressure medium in order to keep a good hydrostatic condition. We performed powder X-ray diffraction measurements at 20 GPa and 40 GPa with increasing temperature up to 523K. Pressure was roughly estimated from the diffraction line position of the sample, which showed that the pressure was 18 GPa at 523 K in the case of 20 GPa at room temperature, and 36 GPa at 523 K in the case of 40 GPa at room temperature. The experimental results show no significant change of the x-ray diffraction profiles of the sample in the both cases, which indicates higher temperature will be required for this study.

[1] A. P. Tsai et al., *Nature (London)* **408**, 537 (2000)

[2] H. Takakura et al., *Philos. Mag. Lett.* **81**, 411 (2001)

Post-CaCl₂ phases Study on GeO₂ at ultrahigh pressures and temperatures

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The studies on post-CaCl₂ phase of SiO₂ have attracted much attention due to its geological, material science, and crystal chemistry interest. High pressure and high temperature experimental results on post-CaCl₂ phase of SiO₂ show large discrepancies between experiments and theories. Tshuchida and Yagi (1989), Andrault et al. (1998), and Ono et al. (2002) reported there is no further phase transformation beyond CaCl₂ structure up to megabar pressure. However, Dubrovinsky et al. (1997) strongly suggested the a-PbO₂ phase was the post-CaCl₂ phase. Theoretical calculations also support this observation, such as Karki et al. (1997) and Teter et al. (1998). Since high P-T experiments on SiO₂ have not produced conclusive solutions so far, an analog material like GeO₂ would be expected to provide the answer at much lower pressures.

The starting material has been examined by x-ray diffraction and confirmed to be a pure α-GeO₂ phase. Then, GeO₂ sample was mixed with Pt powder. The Pt powder served as laser heating absorber and also as internal pressure marker. The mixed sample was loaded into a 90-μm Re gasket hole of a diamond anvil cell. We used Ar as a pressure-transmitting medium and to insulate the sample from diamond anvil. A monochromatic beam with wavelength 0.4131 Å was used to examine the sample and beam size was collimated to 20 μm by 20 μm. Temperature was achieved by employing a continuous multimode Nd:YAG laser with a double-side laser heating technique. The x-ray diffraction patterns of GeO₂ were recorded by an imaging plate.

The GeO₂ sample has been pressurized to ~66 GPa and heated up at about 1000-1500 K. We found α-GeO₂ transform to CaCl₂ phase at pressure above 34 GPa (Fig. 1), which is in accord with previous report [Haines et al. 2000]. Then, a new α-PbO₂ like phase was observed at pressure above 64 GPa and temperature about 1000-1500 K (Fig. 2).

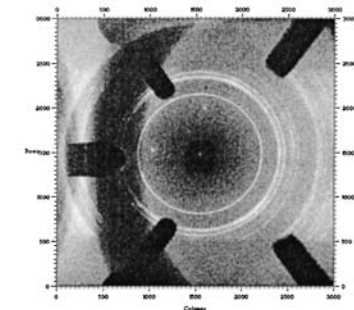


Fig.1 The CaCl₂ phase observed at ~64 GPa.

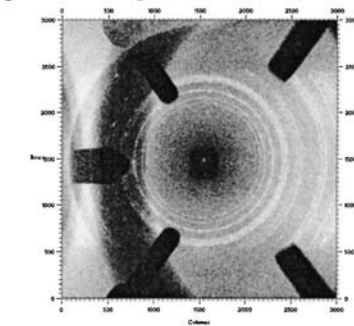


Fig2. The α-PbO₂ like phase observed at ~66 GPa and ~1500 K.