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1. Barium oxide
2. Metallization
3. Diamond anvil cell

The equations of state and the indication of metallization of barium oxide under high pressure

Under high pressure, various materials show changes in crystal structure and electronic states. Some alkaline earth metal oxides are expected to undergo a phase transition from B1 to B2 phases and metallization under high pressure. Calcium oxide (CaO) and barium oxide (BaO) are predicted to metalize above 400 GPa and 230 GPa respectively by ab initio calculation (Tsuchiya&Tsuchiya, 2011, Uludoğan et al., 2001). The phase transitions sequence of BaO is B1→B8→d-B2→B2 and its phase transitions pressure are 5.1 GPa, 19.5 GPa and 120 GPa respectively (Lavanya et al., 2022). The equation of state (EoS) of B2 phase is proposed by ab initio calculation up to 150 GPa, but it has not been proposed for the pressure range where metallization is expected. And, there have been no experimental studies that have confirmed B2 phase of BaO.

Here we conducted static compression experiments of BaO up to 290 GPa using diamond anvil cell (DAC). Lattice constants of BaO were measured by X-ray diffraction experiments at BL10XU in SPring-8 to determine the EoS for the d-B2 and B2 phases. We observed the intensity of transmitted light passing through BaO sample during the compression. If the sample becomes opaque, which is indication of metallization. The pressure in the sample chamber was determined by the EoS of gold (Fratanduono et al., 2021). The EoS parameters of d-B2 and B2 phases were obtained by fitting pressure-volume data to Vinet EoS. According to EoS of B2 phase, the lattice volume is predicted to metalize by ab initio calculation corresponds to 262 GPa. We successfully observed that the gradual decrease in the intensity of transmitted light in the pressure range from 200 to 260 GPa.