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Science Research Bldg. 1, 4th floor.

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Keywords

1. Alkaline earth metal oxide
2. Equations of state
3. Metallization



The equations of state of calcium oxide and barium oxide under high pressure

The phase transition from B1-B2 phase and metallization of alkaline earth metal oxides are expected 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) however, metallization is not confirmed experimentally. The phase transition pressure to B2 phase of CaO and BaO are 67 GPa and 120 GPa respectively, and the equations of state (EoS) of B2 phase are proposed by ab initio calculations up to 200 GPa and 150 GPa respectively (Vyas et al., 2023; Lavanya et al., 2022).

Here we conducted static compression experiments of CaO and BaO up to 350 GPa and 246 GPa using a diamond anvil cell. Lattice volume data of sample and pressure marker were measured by X-ray diffraction experiments at BL10XU in SPring-8 to determine the EoS for B2 phases. The EoS parameters of B2 phases were obtained by fitting pressure-volume data to Vinet EoS. The compression behavior of CaO is consistent with previous experimental study up to 135 GPa (Richet et al., 1988). According to EoS of BaO (B2 phase) and metallization volume predicted by ab initio calculation, metallization pressure of BaO is estimated to be 273 GPa. In BaO, we observed sample became opaque at 242 GPa. However, change of electrical resistance and metallic reflection were not observed up to maximum pressure in these experiments. This result indicates that higher compression is required for the metallization of CaO and BaO.