RAMAN AND X-RAY DIFFRACTION STUDIES ON BAREH9: HIGH VOLUMETRIC CAPACITY HYDROGEN STORAGE MATERIAL

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Abstract

In-situ synchrotron x-ray diffraction up to 32.9 GPa and Raman spectroscopy up to 21 GPa was used to study the structural properties of $BaReH_9$ under pressure. Compression of the initial hexagonal structure (*$P6_3/mmc$*) with lattice parameters a = 5.2882Å and c = 9.3225 Å and a V = 112.891 Å^3 resulted to a 33.4% volume reduction with a lattice parameter a = 4.5735Å and c = 8.3036 and V = 75.209Å^3 at 32.9 GPa. A bulk modulus of K_0 = 23.9 ± 1.0 GPa and a pressure derivative K' = 6.1 ± 0.4 GPa was obtained by fitting of pressure and volume data using obtained using 3rd order Birch-Murnaghan equation of state. The analysis of the x-ray data exhibited a possible orientation disorder in the crystal without any phase transformation in the studied pressure.