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Crystal Structures of and Charge Density Distributions in Perovskite-type Hydrides as a New Series of Hydrogen Storage Materials. K. Ikeda, S. Kato, Y. Nakamori, and S. Orimo, Inst. for Materials Research, Tohoku Univ., Sendai, Japan.

Some ternary hydrides have been reported to exhibit perovskite structures, typically expressed as ABH_3 , and their formation abilities were reasonably explained from the viewpoint of the geometric restrictions on ions, using Goldschmidt tolerance factors ^[1]. In addition, the reversible hydrogen storage abilities have been recently demonstrated for the first time on the hydride ^[2]. For improving the hydrogen storage abilities, it is necessary to clarify the atomistic bonding characters of the hydrides. In this study, the crystal structures and the charge density distributions precisely determined by synchrotron X-ray powder diffraction measurement and its MEM/Rietveld analysis will be presented on the perovskite-type hydrides such as $NaMgH_3$, $CaNiH_3$, and their related systems.

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[1] K. Ikeda, Y. Nakamori, and S. Orimo, *Acta Mater.*, **53** (2005) 3453.

[2] K. Ikeda, Y. Kogure, Y. Nakamori, and S. Orimo, *Scripta Mater.*, **53** (2005) 319.