

中性子回折を用いた $\text{Mg}(\text{OD})_2$ の高温での構造変化の研究 A high-temperature neutron diffraction study on $\text{Mg}(\text{OD})_2$

永井 隆哉^{1*}, 佐野 亜沙美², 飯塚 理子³, 鍵 裕之³
NAGAI, Takaya^{1*}, SANO, Asami², IIZUKA, Riko³, KAGI, Hiroyuki³

¹ 北海道大学・院理, ² 日本原子力研究開発機構, ³ 東京大学・院理
¹Hokkaido University, ²JAEA, ³The University of Tokyo

The structure of deuterated brucite, $\text{Mg}(\text{OD})_2$, was investigated by measuring neutron diffraction at high temperature and at atmospheric pressure to see the dynamic behavior of D atoms with increasing temperature. The neutron diffraction experiments from 202K to 600K were carried out at the beamline of Wide-Angle Neutron Diffractometer (WAND) in the High Flux Isotope Reactor (HRIR), Oak Ridge National Laboratory, USA. Rietveld analysis was performed with both the single D site model and the three-site D model. D atom sits at a crystallographic $2d$ site on the 3-fold rotation axis in the single D site model and at a $6i$ site with occupation factor of $1/3$ in the three-site D model. Analysis for 600 K data was not successful using the single D site model but was successfully converged using the three-site D model. This is possibly due to the strongly anisotropic D motion.

キーワード: ブルーサイト, 重水素原子, 高温, 動的挙動, 中性子回折
Keywords: brucite, Deuterium, high temperature, dynamic behavior, neutron diffraction