High Pressure Effect on Bonding Nature in $KMnF_3$

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Bonding nature between atoms in ABX_3 perovskites is considered to be closely related to their phase instability [1]. The bond length would have primary importance to bonding nature. The bond length can be easily controlled by applying pressure onto the materials. In this study, bonding nature of $KMnF_3$ is investigated by visualizing the charge density distributions under high-pressure.

The synchrotron-radiation powder diffraction experiment was carried out at SPring-8 BL10XU up to 5 GPa under ambient temperature. The pressure-induced phase-transition from cubic to tetragonal phase was confirmed by observing superlattice-reflections at R points, such as (3/2 1/2 1/2), at the vicinity of 3.2 GPa.

The charge-density distributions of the both phases were obtained by the MEM/Rietveld analysis. From the MEM charge densities of the cubic phase, it was revealed that the covalency of Mn-F bond is weakened as the pressure increases. This shows high contrast to the fact that the bond length is shortened as the pressure increases, which is very normal behavior under high pressure. Accompanying these changes under high pressure, the atomic vibration of F atoms perpendicular to the Mn-F bond became greater, which should be related to the softening of rotational mode of the $Mn\text{-}F_6$ octahedron.

[1] Aoyagi S., et al., *J. Phys. Soc. Jpn.,* 2002, **71**, 2353.

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