Poster Presentation

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Phase transition of potassium superoxide KO_2

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Magnetism is one of fundamental phenomena in condensed matter physics and material science. Generally, this magnetic property is found where unpaired electron occupies in d- and f-orbital system of inorganic materials. For instance, magnetism of transition metal oxide with unpaired electron in d-orbital that gives fruitful physical phenomena through interplay between magnetism and other physical properties in superconductivity, colossal magnetoresistance(CMR), multiferroic, etc.

Alkali superoxide AO2(A=K, Rb, Cs) is, so far, rare example of p-orbital quantum molecular magnet that attract researchers whether well-known d-orbital physics can be applicable or not [1, 2]. Two oxygen forms pure O2 molecular dumbbell through covalent bonding between 2p-orbitals. Next, ionic bonding between O2- and A+ induces crystallization of AO2. This crystallization gives one more electron into π* anti-bonding states of O2 molecule that induces quantum magnetism where one unpaired electron occupied in p-orbital inorganic system.

Due to relatively weak ionic bonding compared with covalent bonding of O2 molecular dumbbell, this O2 dumbbell rotation is main origin of structural phase transition, instead of O2 molecule deformation. It was reported that O2 dumbbell rotation induces six structural phases in KO2 [2, 3]. KO2 can be suitable materials for studying dumbbell rotation and p-orbital magnetism.

Nevertheless, room temperature structure is unclear yet [3]. We measured temperature evolution from 4.6 K to room temperature using super-high-resolution neutron powder diffractometer(SuperHRPD) which beamline is installed in MLF, J-PARC. We will discuss detail crystal structure.

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