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 AO$_2$(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 O$_2$ molecular dumbbell through covalent bonding between 2p-orbitals. Next, ionic bonding between O$_2$- and A$^+$ induces crystallization of AO$_2$. This crystallization gives one more electron into π$^*$ anti-bonding states of O$_2$ 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 O$_2$ molecular dumbbell, this O$_2$ dumbbell rotation is main origin of structural phase transition, instead of O$_2$ molecule deformation. It was reported that O$_2$ dumbbell rotation induces six structural phases in KO$_2$ [2, 3]. KO$_2$ 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.


Keywords: Phase transition, p-orbital magnetism, KO$_2$