Abstract of Doctoral Dissertation

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The muon-spin resonance (μSR) and density functional theory (DFT) study of $YBa_2Cu_3O_6$
（$YBa_2Cu_3O_6$ のミュオンスピン緩和法（μSR）および密度汎関数法（DFT）による研究）

The $YBa_2Cu_3O_6$ ($YBCO_6$) is a mother compound of cuprate based high-Tc superconductor. The $YBCO_6$ shows long-range antiferromagnetic ordering and Mott insulator. The long-range AF ordering of this system disappears with doping and superconductivity appears. The detail study of magnetic and electronic state of $YBCO_6$ is very important to understand from which the superconductivity appears. The μSR is extremely sensitive to probe the local magnetism due to the large gyromagnetic ratio of the muon spin. On the other hand, μSR has difficulties in investigating quantitative information of hyperfine interactions due to unknown positions of the injected muon in the materials and complicated local perturbations given by the muon to its surroundings.

The density functional theory (DFT) with the additional Hubbard, U, is employed to muon-site estimation and quantify the muon perturbation. The muon site estimation is based on the local minimum potential as muon has positive charge. The muon then introduced in to the $YBCO_6$ as hydrogen ion. The calculation was done in the large supercell to compensate the behavior of the muon as ultradilute impurity. We found that three distinct muon sites, two near apical oxygen and one near planar oxygen. Our new high-statistics μSR experiment of high-quality single crystal of $YBCO_6$ reveals three distinct muon spin precession components which is consistent with our muon site estimation.

The main parameter that can be inferred from the μSR experiment is internal field at the muon sites. The examination of the internal fields at the estimated muon site was done on the basis dipolar interaction muon and magnetic ion in $YBCO_6$ with considering the local crystal deformation. The internal field calculation by assume the spin reside in the particular ion (point dipole model) is overestimated the internal field at the muon site.

The strong hybridization between *d* orbital Cu with the p orbital O is play the crucial role in the magnetic properties of the cuprates which is known as covalency effect. This phenomena leads to the extension the spin density in the real space which is contradictive with the point dipole model. Since the

long-range antiferromagnetic ordering in the Mott insulator arises from the strong on-site electron repulsive, the spin density has strong dependence to the strength the on-site electron repulsive which is characterized by U value. Thus, the carefully tune of the U value is needed. The best value of the U, 6.7 eV, for the $YBCO_6$ is determined by absolute different the internal field from the experiment and theoretical calculations. The internal field calculation at each muon site on the basis of this model are fairly match with internal fields from the experiment.

It is also found that the ground state of the muon which is referred as zero-point energy (ZPE) vibration motion is play crucial role in the muon site determination. This effect is included simultaneously with covalency effect and local crystal deformation from DFT calculation in order to explain the local internal field at the muon site.