Investigation of muon sites in $YBa_2Cu_3O_6$ using density functional theory†

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Since the discovery of the Cu-based high-*Tc* superconducting oxides, both theoretical and experimental investigations have been carried out to understand their magnetism, electronic properties, and superconducting mechanism. But the mechanism of high-*Tc* superconductivity is still unclear and further investigations are required. The Muon Spin Relaxation (μSR) technique is one of the effective approaches for these investigations. The μSR technique can give us valuable information on high-*Tc* superconductivity, electronic states, spin structures, and hyperfine fields. Additional information on muon sites can also give us more options to quantitatively discuss these properties. Unfortunately, successful determination of muon sites from μSR experimental data has been possible only for few cases in the past. Thus, we have been trying to establish a way to estimate muon sites from a computational view point by using the density functional theory (DFT). We have already tested our method on La_2CuO_4 (LCO) because this system has been well investigated by μSR. There are a lot of experimental data related to the antiferromagnetically ordered state in LCO and we can compare the data with our calculation results to successfully obtain new results in terms of muon sites in LCO.[1)] The similar anitiferromagneticlally ordered state has also been reported in $YBa_2Cu_3O_{6+x}$ (YBCO) and we can apply our computational method to the $YBa_2Cu_3O_6$ as well as the case of LCO.[2-4)]

The hole concentration of YBCO can be controlled by changing the oxygen content, x, from 0 to 1. The system changes from antiferromagnetic state (x = 0) to superconducting state (x = 1). [2-4)] The anti-ferromagnetic transition temperature, T_N, is approximately 350 K at x = 0. Several components of muon–spin precession have been clearly observed below T_N. This indicates that there are some muon sites in YBCO.[6)] In order to optimize the exchange correlation function, we first calculated the density of the state of each electronic orbital of $YBa_2Cu_3O_6$. After optimizing the electronic correlation function, we calculated the electrostatic potential as implemented in Vienna Ab-initio Simulation Package (VASP) by using RIKEN Integrated Cluster of Clusters (RICC) and found six local minimum potential positions. These minimum potential positions can be regarded as initial stopping positions of the injected muons. Three are close to the apical oxygen of the CuO_5 tetrahedra (marked as M1-M3) and one is close to the planar oxygen (marked as M4). [2,6)] The M5 site is close to the Cu(I) site in the Cu-O chain, while the M6 site is between the CuO_2 planes. M5 and M6 are new and different from view point of the well-known argument on the muon-binding state with oxygen because muons prefer to associate with oxygen to form the hydrogen binding state that lowers its potential energy.[5)] According to the following procedure, we estimate the final state of the muon. We put μ^+ on the minimum potential position and recalculate the μ^+ position in the 3x3x3 supercell taking into account the relaxations of the muon and all atomic positions so as to minimize the total energy of the supercell.

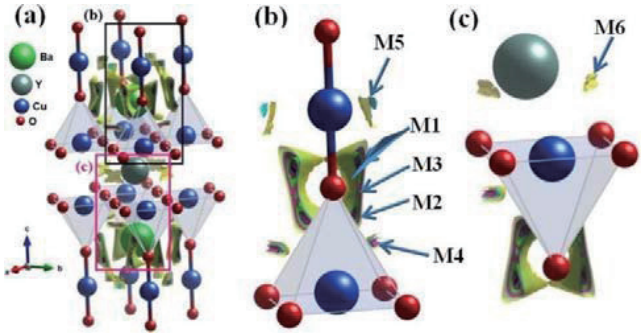

Figure 1. Crystal structure of YBCO with x = 0. Cu(II) in the CuO_2 plane is surrounded by five oxygen atoms and has a spin half. The Cu(II) rules the antiferromagnetically ordered state, while the Cu(I) which is in the Cu-O chain is non-magnetic with a zero spin. We found six local minimum potential positions (M1 to M6) from the calculation by the DFT method. The positions were drawn by the isosurfaces in different colors.

We will carry out precise μSR measurement on YBCO with x = 0 to verify our method for the estimation of muon sites. Then, we will compare the electronic structures, hyperfine fields, and spin structures with the experimental results in terms of insulating YBCO.

References

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