

Study of Implanted Muons in $\text{YBa}_2\text{Cu}_3\text{O}_6$

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Since the discovery of cuprate-based high- T_c superconductivity, enormous efforts in both experimental and theoretical studies have invested to understand its superconductivity mechanism. However, this mechanism is still unclear and debatable. $\text{YBa}_2\text{Cu}_3\text{O}_6$ (YBCO₆) is one of the mother compounds of cuprate-based high- T_c superconductors. This system shows antiferromagnetic (AF) ordering with $T_N = 350$ K.¹⁾ The AF ordering of this system disappears by doping, $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$, and superconductivity appears.²⁾ We study the magnetic and electronic properties of YBCO₆ by using the muon-spin resonance (μSR) technique. This technique is extremely sensitive to probe local magnetism but has a limitation, because muon sites in the lattice and perturbation by muons to the host system are unknown.³⁾

Therefore, we have been developing the method to estimate muon sites in YBCO₆ by using density functional theory (DFT) which is implemented in *Vienna Ab-initio Simulation Package* (VASP). Based on the μSR experimental data of YBCO₆ below T_N , three muon-spin precession components are observed, indicating the presence of three different kinds of muon sites in this system.

We first calculate the density of state and the band structure to confirm the insulator state in this system. Considering strong electron correlation among cuprate ions in this system, we optimize the exchange-correlation function and the value of Hubbard parameter (U). The second step is to calculate the potentials in this system under the same condition as that in the first step. In the calculation of the potential, the pseudopotential for hydrogen is used, because a muon is considered to be a light isotope of a proton. As a muon has a positive charge, it prefers to be located at sites of the local minimum of the potential. Thus the local minimum site can be regarded as the initial muon site. We found three kinds of muon sites (marked M1-M3) in YBCO₆ as shown in Fig. 1.

To investigate the effect of the presence of a muon in the system, we performed calculation by placing a muon at the initial site in the $4 \times 4 \times 2$ supercell and allowing the lattice to be relaxed. Then, we got the final site of the muon, the change of local electronic states and spatial spin distributions.

We are also developing the program to calculate internal fields at the muon stopping sites. In this program, we considered zero point energy (ZPE) vibration of a muon because the muon is a light particle.

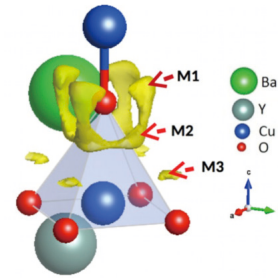


Fig. 1. Possible muon sites in YBCO₆ estimated from our DFT calculations. Yellow area indicates the isosurface at 500 meV.

The density distribution of the muon extends over the amplitude of the ZPE vibration. The density distribution of muon was calculated by solving the Schrödinger equation for the wave function of muon around the local minimum of potential in the range up to 1.5 angstrom. By taking all those results into account, we calculated the internal fields at each kind of muon site to be 116 G for the M1, 335 G for the M2, and 446 G for the M3 sites.

From previous μSR measurements for the antiferromagnetic phase of YBCO, Brewer *et al.* found one muon spin precession frequency in YBCO_{6.2} which corresponds to the internal field 300 G⁴⁾ and Nishida *et al.* found two additional muon spin precession frequencies which correspond to the internal fields of 100–150 G and 1.8 kG. The amplitude of muon spin precession for the 1.8 kG is less than 1%.⁵⁾ The calculated values on the internal fields for the M1 and M2 sites are compatible with the experimental results, 100–150 G and 300 G, respectively. However, the calculated value for the M3 site is not compatible. To clarify the origin of this discrepancy in the values for the M3 site, the μSR measurement for the high-quality YBCO single crystal and further checking the calculation for the M3 site are still ongoing

References

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