μSR remeasurement of La_2CuO_4 to reinvestigate muon sites

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In a previous report,[1)] we have predicted a muon site in La_2CuO_4 (LCO) with the tetragonal structure (the structure above 550 K) by calculating the minimum potential energy for muons, according to the density functional theory (DFT), and the hyperfine field contribution from Cu spins. We predicted two possible muon sites in LCO, although a single muon site with an internal field between 410-430 G was experimentally achieved[2)]. Because of this disagreement, we remeasured the internal field at the muon site using the μSR method with higher statistics. In addition to this experimental effort, we also continued a similar estimation to find all possible minimum potentials in the orthorhombic structure (the structure that occurs below 550 K).

Zero-field (ZF) μSR measurements were performed at the RIKEN-RAL Muon Facility and PSI using a single crystal of LCO in the magnetically ordered state at 10 K and 1.7 K, respectively. The DFT calculation was performed by using the RIKEN integrated cluster of clusters (RICC) system using the Vienna ab-initio simulation package (VASP). A supercell structure that contains 27 unit cells (3×3×3 unit cells) was adopted for calculation taking into account the effect of relaxations of the local lattice and muon positions. The minimum potential in the static case was used to determine the initial positions of lattice points prior to final calculations with relaxation effects. The dipole calculation was performed on the basis of the antiferromagnetic ordered state, which has been experimentally determined by Vaknin et al.[3)] The magnetic moment was traced from 0.10 to 0.70 μ_B/Cu until the dipolar fields fit the internal fields experimentally determined by ZF-μSR.

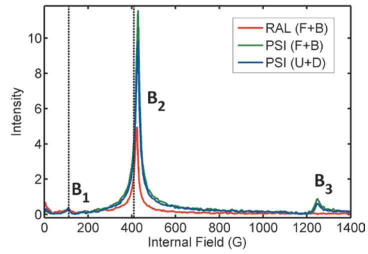

Fig. 1 Fourier spectra of La_2CuO_4 ZF-μSR obtained with high statistics in the RIKEN-RAL and PSI.

Fourier spectra of ZF-μSR are shown in Fig. 1. Three components of internal fields were found. We marked them as B_1, B_2, and B_3 from the lower field component. B_2 has the largest amplitude while B_1 and B_3 have much smaller amplitudes that are less than 1/30 of that of B_2. The internal field of B_2 corresponds to that experimentally observed.[2)] In terms of DFT calculations, three minimum potentials were found in LCO from our current study, as shown in Fig. 2. This result is qualitatively explained by three muon positions in LCO.

We attempted to explain the observed internal fields on the basis of the dipole-dipole interaction by tuning the magnitude of the magnetic moment of the Cu spin. As a result, we found that the three observed components of the internal field can be explained if the magnetic moment of the Cu spin is reduced to be around 0.23 μ_B, as shown in Fig. 3. Such a local reduction of the Cu spin is currently being argued.[4)]

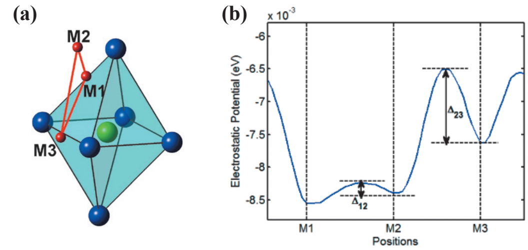

Fig. 2 (a) Minimum potential positions estimated from DFT and (b) shape of the potential energy between minima.

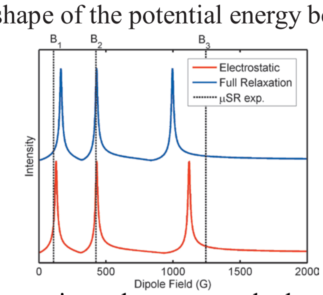

Fig. 3 Comparison between calculated dipolar field spectra and the internal field obtained from μSR experiments.

In conclusion, we found new additional muon sites in LCO from the ZF-μSR experiment with higher statistics. Our DFT calculation supported those three muon sites. Assuming only the dipole-dipole interaction, we suggest the possible local reduction of magnetic moment of the Cu spin to be approximately 50%. The reason for this reduction is currently being discussed.

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