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Anisotropic hyperfine coupling of muonium in CeO₂ studied by muon spin relaxation

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CeO2 is a material that has been widely used in industrial fields such as catalysts and sensors. It is believed that oxygen deficiencies and hydrogen at the deficient positions play an important role in these functions, but the details, including the electronic state, have not been clarified. It has been reported that muons implanted in CeO2 are bound to electrons and form muonium [S.F.J.Cox *et al.*, J. Phys.: Condens. Matter **18**, 1079-1119 (2006)]. However, the sample used in the experiment was a powder, and the information about the oxygen deficiency in the measured sample is unknown. Therefore, we perform the muon experiment using a single crystal sample. By using a single crystal, we can deduce the oxygen deficiency from other measurement technique, and by combining this information with our result of muon experiments, we can clarify the details of the electronic state of hydrogen in CeO2.

It was seen in our muon experiments that muon spin relaxation suggesting the existence of muonium in single crystals of CeO2 appears at temperatures below ~60 K under zero external field. The temperature dependence is qualitatively in good agreement with that reported by Cox *et al.* As the longitudinal magnetic field along the [100] crystalline axis being increased, the spin polarization at t = 0 recovered. It is noted, however, that the obtained magnetic field dependence of the spin polarization at T = 9 K is different from the behavior expected for muonium with isotropic hyperfine coupling, strongly suggesting the anisotropy of the hyperfine coupling constant at the muon stopping site. Furthermore, we observed how the anisotropic behavior seen in longitudinal magnetic fields changes with changing the crystal orientation, taking advantage of the single crystal sample. From these results, we discuss the position of muonium in the crystal lattice and its electronic state.

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