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Anion Configuration of ATaO$_2$N (A=Ba, Sr) Studied by μ-LCR

In perovskite Ta oxynitrides ATaO$_2$N (A=Ba, Sr), a new degree of freedom, $cis/trans$, is introduced by the anion configuration. In these materials, a dielectric constant of about 10^2-10^3 has been observed at room temperature. However, powder X-ray diffractions show structures such as $Pm\bar{3}m$ and $I4/mcm$, which have central symmetry and do not exhibit dielectric polarization [1,2]. Powder neutron diffractions also show structures with similar symmetries, although O/N occupancies have been determined. However, the anion configuration has not yet been determined, and two or three candidate crystal structure models have been proposed [3-5]. On the other hand, first-principles DFT calculations suggest that the most stable structure is a tetragonal crystal, rather than a cubic or tetragonal crystal, and among these, the cis-type of $Pmc2_1$ is the most stable. Taking into account these results, the cis-type of $Pmc2_1$ has been reported to be the most promising candidate [6,7].
This study aims to obtain insight into the O/N configuration from the viewpoint of local structure. Muon cross-resonance (μ-LCR) experiments were performed on powder ATaO$_2$N (A=Ba, Sr) samples. The experiment was performed at S1-ARTEMIS, J-PARC with a magnetic field dependence at 50 K. The muon sites were estimated from Hartree potential calculations by DFT using the ab-initio calculation package VASP.
In addition, the nuclear quadrupole resonance magnetic field of ^{14}N nuclei observed through muons was estimated by calculating the charge density distribution and then performing EFG calculations from the charge density distribution. In my talk, I will show the results observed in μ-LCR and discuss the expected structure.

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