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Mott-insulating state of alkali-metal clusters in sodalite studied by μSR

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In Mott insulators, band electrons are localized due to strong electron-electron interactions. Although the s-electrons of alkali metals are very delocalized, by confining them in the periodic nanospace of zeolite crystals and making them moderately localized, such a strongly correlated electron system can be created.[1] In sodalite, β-cages with an inner diameter of 0.7 nm are arranged in a bcc structure. By loading alkali atoms, an A_4^{3+} cluster (A: alkali atom) is formed in the cage. The cluster has one unpaired s-electron. Antiferromagnetic order of Mott insulating state has been identified in A = Na, K, and K-Rb alloy clusters.[2] T_N systematically increases from 50 K (Na) to 90 K (K-Rb alloy). In ZF-μ^+SR, a uniform local field is observed below T_N, and its value is higher for clusters with heavier chemical compositions.[2]

To clarify the mechanism of the systematic change in the local field and its relation with the Mott-insulating state of this system, we investigate the muon Knight shift by high TF-μ^+SR using NuTime at TRIUMF. We successfully obtained the hyperfine coupling constants between μ^+ and the s-electron above T_N from the $K-\chi$ plot. By combining the ZF-μ^+SR local field,[2] we determined the size of the ordered moments, which systematically decreases from $\simeq 0.5\ \mu_B$ (Na) to $\simeq 0.3\ \mu_B$ (K-Rb alloy). It correlates perfectly with the increase in T_N, namely, the decrease in the electron correlation U/t in the Mott-Hubbard model. From DFT calculations, we found that μ^+ is in a hydride (Mu−) state at the cage center. This also explains that the systematic increase in the local field corresponds to the decrease in U/t due to the shallower potential of the heavier alkali atoms.

[1] T. Nakano and Y. Nozue, Adv. Phys.: X **2**, 254-280 (2017).
[2] T. Nakano *et al.*, J. Phys. Soc. Jpn. **79**, 073707-1-4 (2010).

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