15th International Conference on Muon Spin Rotation, Relaxation and Resonance



Contribution ID: 265 Contribution code: P-THU-19

Type: Poster

Quadrupolar split resonance of ⁸Li in LaAlO₃

Thursday, 1 September 2022 18:40 (20 minutes)

LaAlO₃ is a wide bandgap, transparent oxide commonly used as a substrate for epitaxial film growth and as a vacuum-like electrically insulating layer in heterostructures. Below a soft-mode structural phase transition at about 800 K, it is rhombohedrally distorted from the ideal cubic perovskite structure as the AlO₆ octahedra rotate about the cubic $\langle 111 \rangle$ directions¹. It is a popular substrate, in part, because Al does not support multiple oxidation states like Ni or Ti and because it is well matched to materials such as LaNiO₃ due to the similarity of their lattice constants. Here, we establish the behaviour of ⁸Li in the bulk as a prerequisite to probing the surface effects of the rhombohedral distortion².

We report β -detected NMR of ⁸Li⁺ implanted into a single crystal of rhombohedral LaAlO₃. Like other insulating perovskites³, the resonance is quadrupole split, since even in the cubic phase, its interstitial site (the *P*-site, Wyckoff 3*d* in the cubic phase) is noncubic. In fact, the splitting in the perovskites⁴ is the largest observed for ⁸Li. The splitting is comparably large in LaAlO₃ ($\nu_q \approx 191.3$ kHz), but there is additional splitting due to the rhombohedral distortion.

1. The transition has been studied in some detail by conventional NMR, see e.g., F. Borsa et al, Phys. Lett. A 34, 5 (1971).

2. For example, see the case of SrTiO₃, Z. Salman et al., Phys. Rev. Lett. 96, 147601 (2006)

3. V. L. Karner et al., JPS Conf. Proc. 21, 011024 (2018)

4. This has proven useful for refining the value of the nuclear quadrupole moment, see e.g., A. Voss et al., J. Phys. G: Nucl. Part. Phys. 41, 015104 (2014)

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Session Classification: Posters

Track Classification: Semiconductors