Cation molecular dynamics in hybrid organic-inorganic perovskite MAPbI₃: Reanalysis of the µSR study

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Organic-inorganic hybrid perovskites (HOIPs) are materials with a structure in which organic molecules are confined in a perovskite lattice and have been intensively studied in recent years as the next generation photovoltaic compound. It has been reported that an energy conversion efficiency is approximately 25%, which is comparable to those of current siliconbased solar cells. Several theories have been proposed as to the reason for the high conversion efficiency. In particular, we have focused on the relationship between the lifetime of photoexcited carriers and the dynamic behavior of organic molecules in this material, probed by the muon spin rotation/relaxation (µSR) technique. Previously, we found that in MAPbI₃ and FAPbI₃, representative HOIPs, the remarkable temperature dependence of the muon spin relaxation rate can be quantitatively explained by changes in the rotational motion of organic molecules, and that the temperature dependence of the lifetime of photoexcited carriers is in good agreement with that of the muon spin relaxation rate, suggesting that the local dielectric constant due to organic molecules may play a key role in the lifetime of photoexcited carriers [1, 2]. Very recently, Ito and Kadono studied the analysis of the µSR time spectra considering contributions from multiple dynamic magnetic moments and tried to analyze the results of FAPbI₃ as an example [3]. As a result, they successfully extracted the motions of organic molecules from the µSR experimental results. In the present study, this method will be applied to the experimental results of MAPbI₃ to gain further insight into the dynamic behavior of organic molecules.

References

[1] A. Koda et al., PNAS **119**, e2115812119 (2022).

[2] M, Hiraishi et al., J. Appl. Phys. 134, 055106 (2023).

[3] T. U. Ito and R. Kadono, J. Phys. Soc. Jpn. 93, 044602 (2024).