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IT-5-P-1793 Measurement of liquid vibrational spectra using monochromated STEM-EELS

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Liquid is widely used in daily life and industrial activities. The dynamic behavior of the molecules in liquid is an important factor to determine the various liquid properties. The dynamic behavior of liquid molecules has been extensively investigated using infrared (IR) spectroscopy and Raman spectroscopy. However, these spectroscopy techniques allow us to obtain only averaged information of the entire sample. On the other hand, a specific location, such as solid-liquid interface, plays important role for reactions in electrochemistry and organic chemistry, in which liquid is treated as reactants and reaction media. That is, the methods for analyzing the dynamic behavior of liquid molecules at high spatial resolution have been desired.
In this presentation, thus, we will report the results of the measurements of liquid vibrational spectra by monochromated STEM-EELS. For the analyses, I used an aberration corrected STEM with a monochromator (JEM-2400FCS, JEOL Ltd., 120keV). The energy resolution reached 0.065eV using the monochromator. As a liquid sample I chose a popular ionic liquid, 1-ethyl-3-methylimidazolium bis (trifluoromethyl-sulfonyl) imide (C2mim-TFSI). In order to verify the vibrational spectra by STEM-EELS, an IR spectrum was measured from the same sample. In addition, first principles calculations were performed to interpret the peaks in the vibrational spectrum. The plane-wave pseudopotential method (CASTEP code) was used in the calculations.
From the STEM-EELS measurement, the HOMO-LUMO gap of C2min-TFSI was estimated to be 5.3eV, which is consistent with the results of the first-principles calculations and a separately measured ultraviolet-visible (UV-vis) spectrum. The peaks ascribed to the molecular vibration were measured in the vicinity of 0.4eV. These peaks were also observed in the IR spectrum and the one from the first-principles calculations. From those analyses, it was confirmed that the peaks at the 0.4eV correspond to the CH bonds stretching peaks. Based on this study, we have demonstrated that the vibrational peaks of the nano area in liquid are available by the monochromated STEM-EELS.

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