Water dynamics of zirconium oxide nanofluid

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Fluids with nanoparticles dispersed in a liquid are called nanofluids and are expected to be new heat-conductive materials. Some nanofluids show higher thermal conductivity than the theoretical value predicted by the Maxwell-Garnett equation. The dynamics around nanoparticle is different from that of bulk liquid. Hence, the thermal conduction of nanofluid might be affected by the dynamics of liquid. The water-based zirconium oxide (ZrO_2) nanofluid targeted in the present study exhibits high thermal conductivity, stability, and high safety (inflammable), so it is expected to be a high-performance thermal conductive material. The translational motion of water in ZrO_2 nanofluid was investigated using DNA spectrometer at J-PARC [1]. To clarify the mechanism of enhanced thermal conductivity of nanofluids from the viewpoint of liquid dynamics, it is important to observe both translational and rotational diffusion of water molecules over a wide temperature range. AGNES spectrometer is suitable for the investigation of faster dynamics. The QENS of water-based ZrO_2 nanofluids at 20 and 30 wt% and H_2O was investigated at the temperature range of 278-298 K.

ZrO_2/water nanofluid exhibits a pH of around 5. Therefore, the sample was placed in the gap of a double-cylinder glass cell, which was then sealed in an aluminum cylindrical cell. The scattering intensity of water is high, and to prevent multiple scattering, the transmission of the sample was 90% or higher. To observe a wide dynamics range, QENS spectra was measured with both 120 μeV (standard mode: ST) and 50 μeV (high-resolution mode: HR) energy resolutions. The Q range is 0.38-2.63 $Å^{-1}$ (ST) and 0.29-2.03 $Å^{-1}$(HR). Dynamic structure factors obtained from quasi-elastic scattering measurements are fitted with one delta and one Lorentzian function.

As shown in Figure 1, the half-width half-maximum of quasi-elastic component of QENS spectra of 20 wt% nanofluid is similar to that of pure water. That of 30 wt% nanofluid is slightly smaller than that of pure water. This implies that the water dynamics around nanoparticles is slow compared with bulk water. The same result is seen at 278 and 288 K. It is consistent with the results investigated by DNA spectrometer and NMR [1].

The difference between the nanofluid and the bulk water was very small. This is because the contribution from bulk water is large in the nanofluid. A molecular dynamics simulation of the nanofluid should be performed to separate the contribution of water dynamics near the surface of the nanoparticle from that of bulk water.

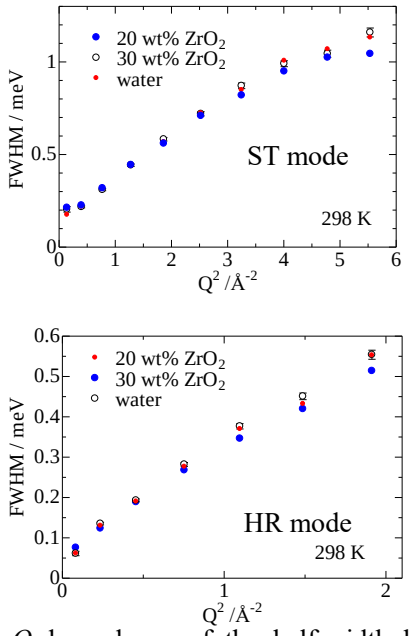

Fig. 1. Q-dependence of the half-width half-maximum of quasi-elastic component of the spectra (standard and high-resolution modes) for ZrO_2 nanofluid.

[1] K. Yoshida et al, J Mol. Liquids 366, 120218 (2022).