H-H, H-X, and X-X partial structure factors in concentrated NaFSA-propylene carbonate solutions

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Recently, structure of concentrated Na-salt solutions dissolved in liquid propylene carbonate (PC) has been received much attention as possible electrolyte solutions for the next generation high performance sodium ion batteries. In principle, structural characteristics of solvated sodium ion can be deduced from diffraction techniques. However, detailed structural analysis of the solvated sodium ion is extremely difficult because of a larger size and rather complicated structure of solvent PC molecule. Neutron diffraction with H/D isotopically substituted samples has a potential to distinguish H-H, H-X and X-X (X: atom(s) except for hydrogen). In the present study, neutron diffraction measurements on H/D isotopically substituted 10 mol% NaFSA (FSA^-: $N^-(SO_2F)_2$) solutions (H:D = 2:98 ($b_H = b_D$), 64:36 (b_H = 0) and 67:33 ($b_H = b_D/2$)) to obtain structural information on the solvated sodium ion in organic carbonate solutions. Neutron diffraction measurements have been carried out using the 4G (GPTAS) spectrometer installed at JRR-3 research reactor operated at 20 MW, JAEA, Tokai, Japan. Incident neutron wavelength, λ = 1.106 Å, has been determined from Bragg reflections of KCl powder. After corrections for instrumental background, absorption in sample and cell, the count rate observed for the sample solution has been converted to absolute scattering cross section by using corrected observed scattering intensity from standard vanadium rod (10 mm in diameter). The self-scattering intensity of sample solution involving the inelasticity contribution has been estimated by a polynomial function of Q (= $4\pi \sin\theta/\lambda$, θ: scattering angle) and the sum of intramolecular interference terms for PC and FSA^- have been subtracted from observed scattering cross section to deduce the intermolecular interference term, $i^{\mathrm{inter}}(Q)$. H-H, X-H and X-X partial structure factors, $a_{ij}^{\mathrm{inter}}(Q)$, have successfully been obtained by combining intermolecular interference terms observed for the D, ^{0}H and $^{0\text{-}2}$H sample solutions. Corresponding intermolecular partial distribution functions are obtained from Fourier transform of observed $a_{ij}^{\mathrm{inter}}(Q)$. Fig. 1 represents H-H, X-H and X-X intermolecular partial structure factors observed for 10 mol% NaFSA-PC solutions, respectively. Detailed structure parameters for the solvated sodium ion, $Na^+(PC)_n$, can be deduced by the simultaneous least squares fitting analysis of the observed $a_{ij}^{\mathrm{inter}}(Q)$ functions. Further data analyses are in progress.

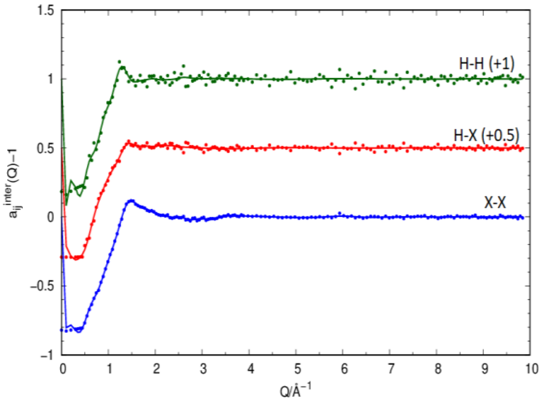

Fig. 1. H-H, X-H and X-X intermolecular partial structure factors observed for 10 mol% NaFSA-PC solutions.