Experimental report

17/03/2021

Proposal: **6-02-618**

Council: 10/2020

Title: Influence of HFE on the dynamics of an ionic liquid electrolyte

Research area: Materials

This proposal is a new proposal

Main proposer: **Filippa LUNDIN**

Experimental team: Peter FALUS

Local contacts: Peter FALUS

Samples: 1-Butyl-1-Methylpyrrolidinium bis(fluorosulfonyl)imide (P14FSI) : Lithium bis(fluorosulfonyl)imide (LiFSI) : 1,1,2,2-Tetrafluoroethyl 2,2,2-Trifluoroethyl Ether (HFE)

Instrument	Requested days	Allocated days	From	To
WASP	5	4	15/02/2021	19/02/2021

Abstract:

We propose to investigate the dynamics in a new electrolyte system, a localised highly concentrated electrolyte, where the viscosity is lowered by a diluent while locally preserving a highly concentrated ionic environment. The aim is to investigate how the dilution of an ionic liquid electrolyte affects the local dynamics and the microscopic conduction mechanism and link it to the behaviour of the macroscopic conductivity. With neutron spin echo spectroscopy at WASP we can directly access the time scales of local dynamics (ps-ns) at relevant length scales of charge correlation in these liquids.

Influence of HFE on the dynamics of an ionic liquid electrolyte

Experimental report

Virtual beamtime 15-19/2 - 2021

Proposal number: 6-02-618
Main proposer: Filippa Lundin
Co-proposer: Aleksandar Matic
Local contact: Peter Falus
Instrument: WASP

In this experiment we investigate the dynamics in diluted highly concentrated electrolytes. A diluent is added to lower the viscosity of the highly concentrated electrolyte while preserving the favourable properties related to strong ion correlations. The aim is to correlate the local dynamics on length scales of charge correlations, accessed by the WASP spectrometer, and macroscopic ion transport.

The investigated system consist of the ionic liquid $Pyr_{14}FSI$ (1-butyl-1-methylpyrrolidinium bis(fluorosulfonyl)imide) doped with the Li-salt LiFSI, diluted by the fluorinated ether HFE (1,1,2,2-tetrafluoroethyl 2,2,2-trifluoroethyl ether) at the $Pyr_{14}FSI$:LiFSI:HFE molar ratios 1:0.2:0, 1:0.2:0.5 and 1:0.2:1. Hydrogenated materials were used and the scattering is dominated by incoherent scattering from the cation, Pyr_{14}, of the ionic liquid in all samples (>75% of the scattering even at high HFE concentrations). A wavelength of 7Å (6 ps-6 ns and Q=0.6-1.6$Å^{-1}$) was used to cover the full range of cation motions and length scales found in previous experiments on a neat ionic liquid with the same cation[1].

Figure 1 (left) shows the normalised intermediate scattering function obtained in the experiment for the different samples at two temperatures. It is clear that with the WASP spectrometer provides good data quality and that we can clearly capture the dynamics in all samples. As expected for liquids, a strong temperature dependence is found for the dynamics which spans over the whole time-window (almost 4 orders of magnitude) covered by the WASP spectrometer. Looking at the different concentrations there is a distinct difference between the samples containing HFE and the sample that does not. From a first preliminary analysis we can qualitatively correlate the local dynamics with the macroscopic conductivity, i.e. faster dynamics with the introduction of HFE to the system. The right figure shows the normalised intermediate scattering function from the $Pyr_{14}FSI$:0.2LiFSI sample for different Q-values, revealing a strong Q-dependence in the investigated region, a signature of diffusive motion.

A detailed analysis of the spectral shape, i.e. the nature of the relaxation function, will be performed in order to identify the detailed nature of the relaxation processes contributing to the scattering. The results from the WASP experiment will be combined with data from diffusion NMR and conductivity in order to span from local molecular/ionic relaxations to macroscopic ion conductivity in order to better understand ion transport in the diluted highly concentrated electrolyte system.

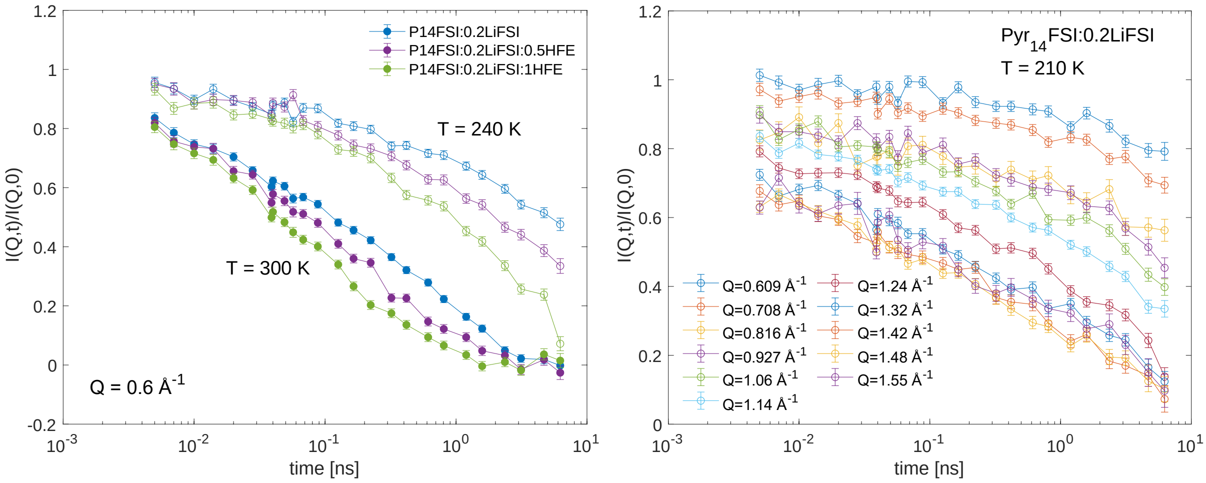

Figure 1 Normalized intermediate scattering function for (left) different HFE concentrations at two temperatures measured at Q=0.6 Å^{-1} and (right) different Q-values for $Pyr_{14}FSI$:0.2LiFSI at 210K.

1. Lundin, F. *et al.* Pressure and Temperature Dependence of Local Structure and Dynamics in an Ionic Liquid. *J. Phys. Chem. B* (2021) doi:10.1021/acs.jpcb.1c00147.