Experimental report

02/11/2015

Proposal:	**9-10-1342**	**Council:**	4/2014
Title:	Unraveling Dynamical Motions in Cationic Micelles		
Research area:	Soft condensed matter		

This proposal is a new proposal

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Samples:
D_2O
$C_{14}H_{29}N(CD_3)_3Br$
$C_{14}D_{29}N(CH_3)_3Br$
$C_{14}H_{29}N(CH_3)_3Br$

Instrument	Requested days	Allocated days	From	To
IN16B	3	3	14/11/2014	17/11/2014

Abstract:

Quasielastic Neutron Scattering (QENS) study in various micellar systems performed by us showed two distinct motions namely global and internal motion. Molecular dynamics (MD) simulation results also confirmed the same and further predicted that the internal motion is dominated by the effect of 'hydrophobic glue', which holds the micelle together and is most effective in the middle regions of the chains while the head groups and tails, to a lesser extent. In order to verify this and investigate the selective segmental dynamics, we have carried out QENS study on fully protonated and partially deuterated viz. 1) head group deuterated and 2) tail deuterated Tetra trimethylammonium Bromide (TTAB) micelle using IRIS spectrometer in which both segmental and global dynamics contribute. As the global motion involves both translation as well as rotation of the whole micelle, the effect of them in partially deuterated samples would be different, therefore high resolution data is essential to probe the existing dynamical behavior.

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Unraveling Dynamical Motions in Cationic Micelles

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Amphiphilic molecules such as surfactants and lipids undergo self-association under specific conditions to form aggregates such as micelles, vesicles, bilayers, wormlike micelles, etc. Self assembled micellar aggregates have been the subject of intense interest for several decades, both from a fundamental physical-chemistry point of view and because of their widespread applications in detergent, cosmetic, pharmaceutical and food industries. While understanding of structure and macroscopic behavior seems to converge, the dynamical behavior of these assemblies and their correlation with microstructure is of current interest. Local dynamics in such assemblies are important in understanding various functions such as release of solubilized drugs, micellar breaking and synthesis of nano-particles with most relevant processes being initiated at the micelle surface.

Dynamical processes in micelles are complex and include multiple relaxation processes on local and global scales. We have carried out measurements on anionic as well as cationic micelles in a wide dynamical range using various instruments to elucidate various dynamical processes that could present in these molecular self assemblies. Combining the data obtained from TOF spectrometers IN5, IN6 at ILL, Focus at PSI and backscattering spectrometer IRIS at ISIS facility, we have obtained detailed dynamical landscape in different ionic micellar systems [1]. Charged spherical micelles can grow into elliptical rod like structures by addition of electrolytes that screen the electrostatic repulsion [2,3]. Such changes in shape and size are expected to affect the global dynamics of the micelle significantly. We have carried out QENS measurements on micelles based on SDS surfactant using IN16B with and without addition of NaCl electrolyte to see the effect on global dynamics exclusively, as it is expected that the fast internal motion would be beyond the energy window of IN16B, but the global motion being a slower will be observed without ambiguity.

Figure 1 shows the data after the contribution from the solvent (D_2O) and empty can are removed. Though it is found that with the addition of salt the QE broadening is reduced but the effect is not very significant as expected from the structure studies [.

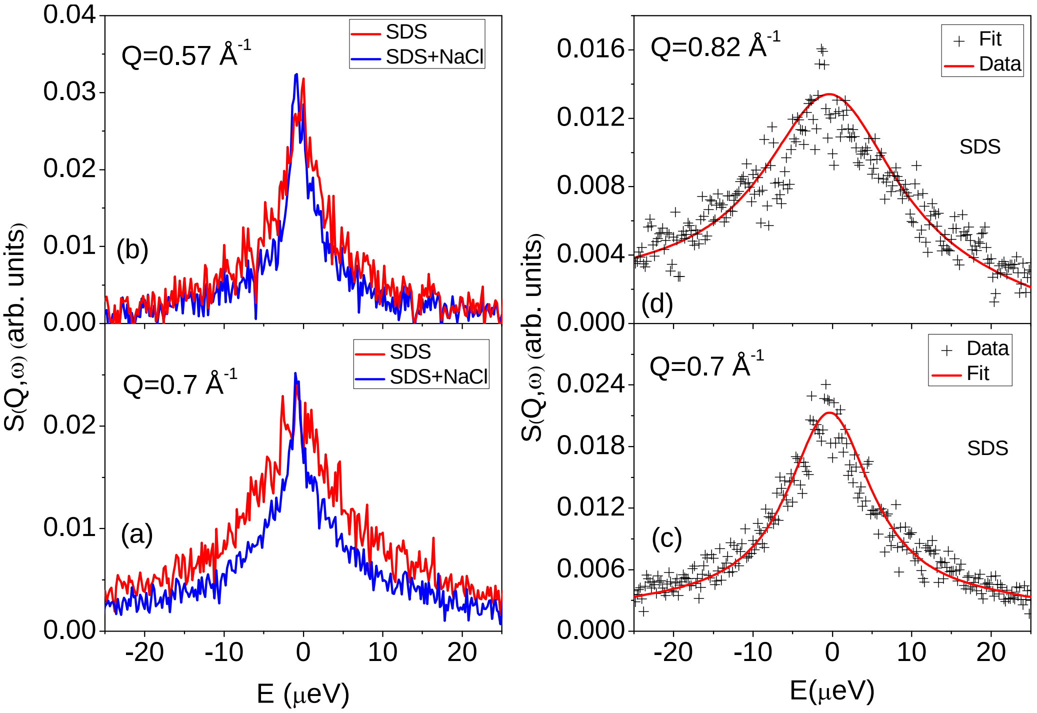

Fig. 1 *QENS data for SDS and SDS+NaCl a) at Q = 0.7* $Å^{-1}$ *and b) at Q = 0.57* $Å^{-1}$. *QENS data with a Lorentzian function fit for SDS micelle at c) Q = 0.7* $Å^{-1}$ *and b) at Q = 0.82* $Å^{-1}$.

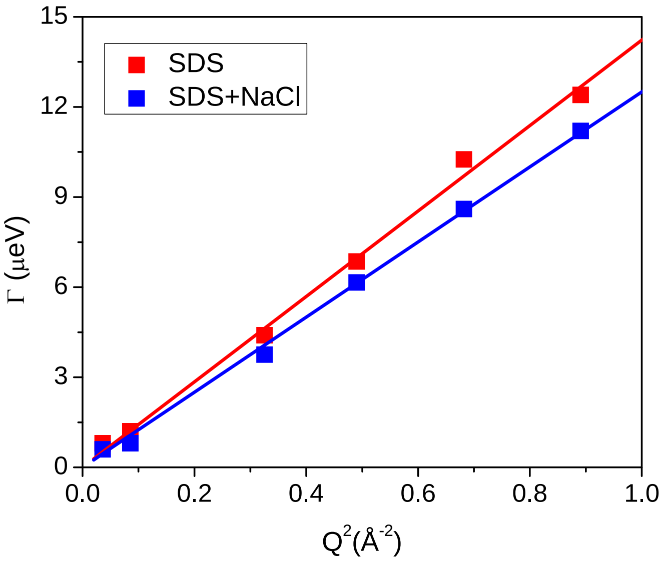

Fig. 2 *Variation of the half width at half maxima (HWHM) of the QE broadening. Straight lines are calculated as* DQ^2 *law.*

QENS data are fitted with a single Lorentzian in order to estimate the behavior quasielastic width with Q. Fitted data for SDS micelle at some typical Q values are shown in Fig. 1c and

Fig. 1d. Fig. 2 shows the behavior of half width at half maximum of the Lorentzian with Q^2. Diffusivity corresponding to global motion estimated for SDS and SDS+NaCl are 2.2×10^{-6} cm^2/sec and 1.9×10^{-6} cm^2/sec respectively.

[1] V. K. Sharma, Gunjan Verma, S. Gautam, P. A. Hassan, S. Mitra and R. Mukhopadhyay, *J. Phys. Chem. B* **114** (2010) 17049; S. Mitra, V. K. Sharma, V. G. Sakai, J. Peter Embs and R. Mukhopadhyay, *J. Phys. Chem B*, **115** (2011) 9732; V.K. Sharma, S. Mitra, V.G. Sakai, P.A. Hassan, J. Peter Embs and R. Mukhopadhyay, *Soft Matter*, **8** (2012) 3151**;** V. K. Sharma, S. Mitra, V.G. Sakai and R. Mukhopadhyay, *J. Phys. Chem. B* **116** (2012) 9007; V. K. Sharma, S. Mitra, M. Johnson and R. Mukhopadhyay, *J. Phys. Chem.* B **117** (2013) 6250; B. Aoun, V.K. Sharma, E. Pellegrini, S. Mitra, M. Johnson and R. Mukhopadhyay, *J. Phys. Chem.* B, **119** (2015) 5079

[2] S.S. Berr, R.R. M. Jones, Langmuir, **4** (1988), 1247

[3] G Garg, P.A. Hassan, V.K. Aswal, S.K. Kulshreshtra, J. Phys. Chem. B, **109** (2005) 1340.