Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Structure and Dynamics of Cellulose Molecular Solutions
HOWARD WANG, XIN ZHANG, University of Maryland, College Park, MADHUSUDAN TYAGI, YIMIN MAO, NIST Center for Neutron Research, ROBERT BRIBER, University of Maryland, College Park — Molecular dissolution of microcrystalline cellulose has been achieved through mixing with ionic liquid 1-Ethyl-3-methylimidazolium acetate (EMIMAc), and organic solvent dimethylformamide (DMF). The mechanism of cellulose dissolution in tertiary mixtures has been investigated by combining quasielastic and small angle neutron scattering (QENS and SANS). As SANS data show that cellulose chains take Gaussian-like conformations in homogenous solutions, which exhibit characteristics of having an upper critical solution temperature, the dynamic signals predominantly from EMIMAc molecules indicate strong association with cellulose in the dissolution state. The mean square displacement quantities support the observation of the stoichiometric 3:1 EMIMAc to cellulose unit molar ratio, which is a necessary criterion for the molecular dissolution of cellulose. Analyses of dynamics structure factors reveal the temperature dependence of a slow and a fast process for EMIMAcs bound to cellulose and in DMF, respectively, as well as a very fast process due possibly to the rotational motion of methyl groups, which persisted to near the absolute zero.

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Date submitted: 06 Nov 2015 Electronic form version 1.4