Quasielastic neutron scattering investigation of supercooled water confined in nanoporous silica matrices—liquid-liquid transition

[1]A. Faraone, [1]L. Liu, [2]C-Y. Mou [2]C-W. Yen and [1]Sow-Hsin Chen

[1]Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

[2]Department of Chemistry, National Taiwan University, Taipei, Taiwan 106

Using incoherent quasielastic neutron scattering we investigated the dynamics of water confined in two nanoporous alumino-silicate matrices, from ambient temperature down to deeply supercooled states in a temperature range inaccessible in bulk water. We collected data using three instruments with widely different resolutions, the Fermi chopper, the disk chopper, and the backscattering spectrometers, at the NIST Center for Neutron Research. The confining systems were lab synthesized mesooporous silica MCM-41-S with cylindrical pores of 14 to 20 Å diameter. Inside the pores of these matrices the freezing process of water is strongly suppressed, taking place at a temperature about 60 K less than in bulk water. Thus, with the combined use of different instruments, we were able to study an interesting temperature range, 220 K <·T <·300 K. The data from all the three spectrometers were analyzed using a single consistent intermediate scattering function of water based on the relaxing cage models for the translational and rotational motions.

We observe a clear evidence of a cusp-like dynamic transition, which can be described as a fragile-to-strong liquid transition. The transition temperature decreases steadily with an increasing pressure, tracking the homogenous nucleation temperature line of bulk water, until it intersects this line at a pressure 1.6 kbar and at a temperature 200 K. Above this pressure, the cusp-like transition disappears and it is no longer possible to identify the characteristic feature of the fragile-to-strong transition.

References:

[1] Faraone A, Liu L, Mou CY, Shih PC, Brown C, Copley JRD, Dimeo RM, Chen SH, 2003, "Dynamics of supercooled water in mesoporous silica matrix MCM-48-S" *European Physical Journal E* 12: S59-S62 Suppl. 1

[2] Liu, Li, Antonio Faraone and S.H. Chen, 2002 "A Model For the Rotational Contribution to Quasi-elastic Neutron Scattering Spectra From Supercooled Water," *Phys. Rev. E*. 65, 041506-8.

[3] L. Liu, A. Faraone, C.-Y. Mou, P.-C. Shih, and S.-H. Chen, 2004, "Slow dynamics of supercooled water confined in nanoporous silica materials" *J. Phys. Condensed Mat*, 16, S 5403-5436

[4] Faraone, A., Li Liu, Chung-Yuan Mou, Pei-Chun Shih, John R.D. Copley, and Sow-Hsin Chen, 2003 "Translational and rotational dynamics of water in mesoporous silica materials: MCM-41-S and MCM-48-S," *J. Chem. Phys*. **119**, 3963-3971.

[5] A. Faraone, L. Liu, C.-Y. Mou, C.-W. Yen, and S.-H. Chen, 2004, "Fragile-to-Strong liquid transition in deeply supercooled confned water" *J. Chem Phys*., 121, 10843.

E-Mail: cymou@ntu.edu.tw
Website: http://www.ch.ntu.edu.tw/faculty/new93/cymou-c.htm