Supercooled Water Confined in a Silica Xerogel: Temperature and Pressure Dependence of Boson Peak and of Mean Square Displacements

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Abstract

A silica xerogel can be obtained from an alcoxide precursor (TMOS, tetramethylortosilcate) via the sol-gel method: TMOS hydrolysis and subsequent polycondensation yields a solid, disordered, porous SiO2 matrix (average pore dimensions ~20Å). Inside the pores water is trapped and the hydration level h=gr[H2O]/gr [SiO2] can be easily controlled.

The presence and temperature dependence of the boson peak (BP) in xerogel confined supercooled water was studied with inelastic neutron scattering (spectrometer IN6 at ILL, Grenoble) in xerogel samples having h=0.4 and h=0.2. After careful subtraction of the contributions arising from the matrix and from quasi-elastic scattering, the BP contribution was analysed in terms of a log-normal distribution to obtain the excess density of states (DOS). A clear inversion in the temperature dependence of the peak height of the excess DOS was observed at about 225K, the same temperature as the proposed LDL->HDL transition in supercooled water.

The pressure dependence of mean square displacements (MSD) was investigated, in the same samples, with elastic neutron scattering (spectrometer IN13, at ILL,Grenoble), exploiting the high pressure cell developed by J. Peters and collaborators. At 250K, a marked MSD increase with pressure was observed, in agreement with the well known "anomaly" of supercooled water and with previous experimental results. However, at 210K the pressure effect was much lower, again in agreement with the presence of an LDL->HDL transition in supercooled water.

Finally, the relevance of the above results to protein dynamics and in particular to the "protein dynamical transition" will also be discussed.