Confined Water (1992)

Single particle dynamics of hydration water in protein, M.C. Bellissent-Funel, J. Teixera, J.F. Bradley, S.H. Chen and L. Crespi, Physica B 181 &181, 740 (1992).

Comment by Wolfgang Doster at bioneutron.de

Marie Claire and S. Chen picked up the sample and the scientific approach of H. Middendorf about ten years later. H_2O is studied absorbed by perdeuterated C-phycocynin. The old paper of Middendorf was not cited however. The authors perform a decent dynamic analysis of the neutron scattering spectra at different temperatures again with a striking result concerning the Q-dependent line-width: The width of the hydration water spectrum, in contrast to bulk water, levels of below Q = 1 A^{-1}. (black dots). There is even a well-defined cross-over at Q = 1 A^{-1}. The conclusion is: The protein hydration water is "confined" by the protein. This seems a great application of the Dianoux-Volino model: The water performs a free diffusion inside a solid sphere of a given size (cross-over). A Gaussian confinement in a harmonic potential does not have an upper limit and does not lead to a low Q plateau. What is wrong?

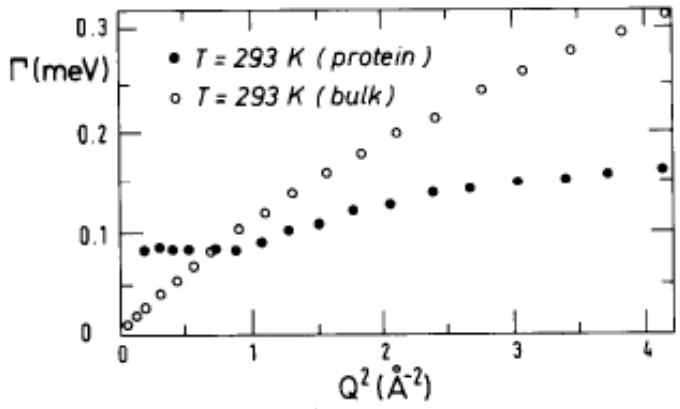
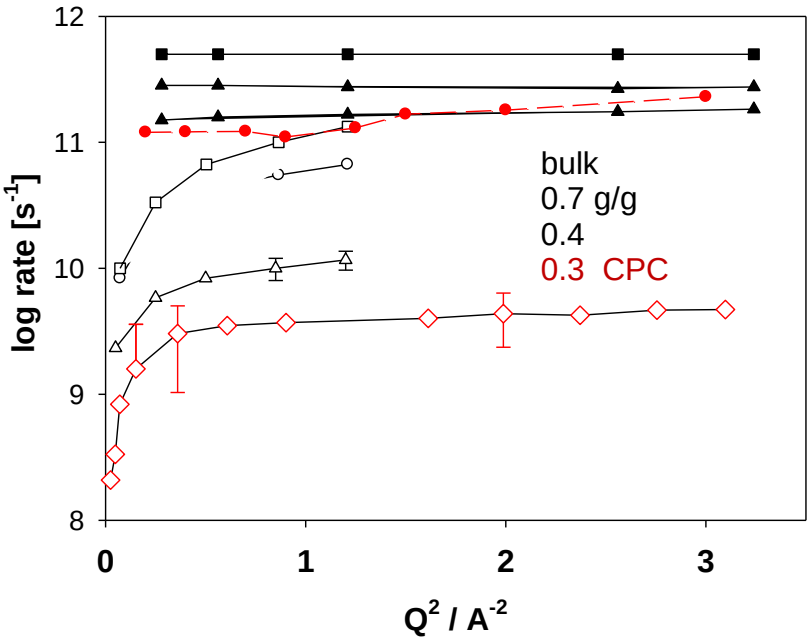


Fig. 4. HWHM of the Lorentzian quasi-elastic line Γ versus Q^2, for $T = 293$ K.

The full red points in the figure below were taken from the above study (Doster, BBA 2005,



and Doster et al (Phys.Rev. Lett 2010)). The black points (open and full) were derived from our spectral analysis of H_2O hydrated myoglobin at various degrees of hydration (BBA 2005). The spectrum contains two components, broad from rotation and narrow from translation. The rotational width is independent of Q. The translational width goes with Q^2 at low Q (diffusion) and saturates at high Q due to the cage effect (Settles /Doster, Faraday Discussion 103, 1996).

Bellissent-Funel et al thus confused the fast Q-independent process of water reorientation with the slower translational diffusion, which they could not resolve in their experiment. There is no plateau at low Q!

Protein hydration water is thus not confined, which is a basic result of neutron scattering! The DV model does not apply, if it does, there is probably something wrong with data. As already mentioned in my comment on Middendorfs work, low Q spectra are prone to artefacts such as multiple scattering or the vanishing incoherent cross section of the sample at low Q.

I am discussing this error because Jose Teixera brought it up recently without corrections at a Les Houches seminar (2013) as a proof of confined hydration water. The special properties of protein hydration water were first brought up by Settles et al in (1996) Faraday Discussion 103.