

A model for water motion in crystals of lysozyme

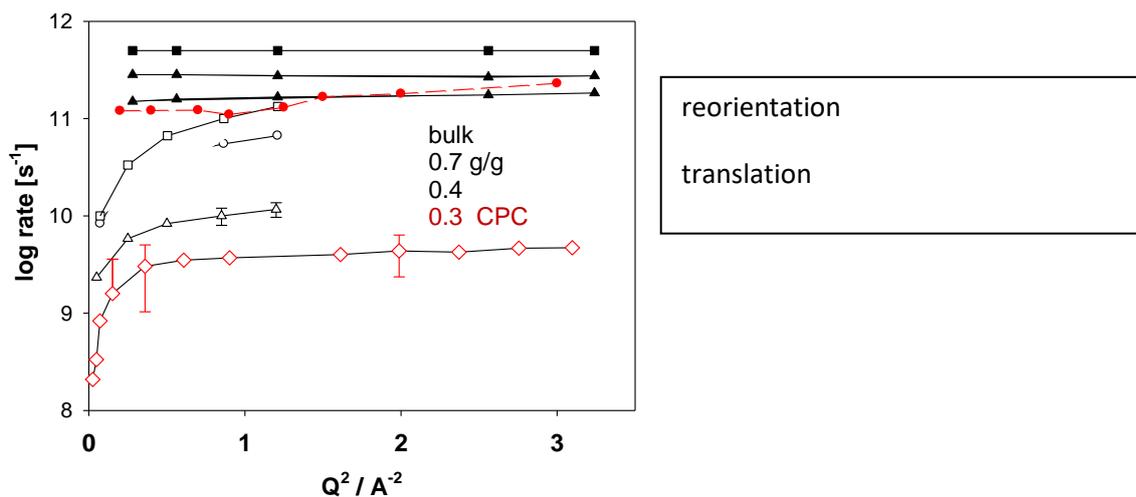
by C. Bon , Dianoux, Ferrand, Lehmann.

Biophys. (2002) 83, 1978

Comment by Wolfgang Doster at bioneutron.de

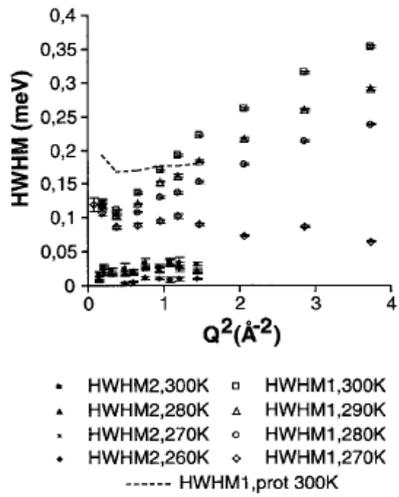
This study was performed by experts of X-ray and neutron scattering. A full dynamic analysis of the spectra is presented at high level. Their model was however inappropriate and led to the odd conclusion, that water near the protein surface moves faster than interstitial water, suggesting some channeling. Biological applications in the cell were imagined.

This paper has the same deficiency as the Bellissent study in 1992 (see Confined Water I): The instrumental resolution was not sufficient to resolve the translational diffusion of crystal water: The quasi-elastic spectrum of water is not Lorentzian, it can be decomposed into two components, (1) reorientational motion, linewidth about 0,1 -0,2 meV (5-10 ps) independent of the wave vector Q and (2) translational diffusion on a scale of nanoseconds (0,02 meV), which is Q-dependent. The first figure below shows the two components derived for bulk water and hydration water of myoglobin and phycocyanin at different degrees of hydration (Doster, Settles BBA 2005, Doster et al. PRL (2010)).



The lower figure shows the results of C. Bon: again two components are derived, which are both identified with translational diffusion. The low-Q plateau of the fast component is again interpreted by the Dianoux-Volino (DV) model of free diffusion inside a solid sphere. The Q-dependent width is most likely an artefact of the unconstrained fitting procedure of amplitude ($\sim Q^2$) and width.

fast DV confined diffusion of water
near the protein surface



slow „interstitial“ diffusion of water in the crystal

fig. 2: Le Bon et al.: two components: I have never seen a convincing application of the DV model.

diffusion of confined water

diffusion of interstitial water