Protein Dynamical Transition at 110 K? By Kim et al PNAS 2011

Proteins are known to undergo a dynamical transition at around 200 K but the underlying mechanism, physical origin, and relationship to water are controversial. Here we report an observation of a protein dynamical transition as low as 110 K. This unexpected protein dynamical transition precisely correlated with the cryogenic phase transition of water from a high-density amorphous to a low-density amorphous state. The results suggest that the cryogenic protein dynamical transition might be directly related to the two liquid forms of water proposed at cryogenic temperatures.

Comment by Wolfgang Doster at bioneutron.de

The authors use the term “dynamical transition” to characterize changes in static molecular disorder as a result of a structural change, presumably the HDA to LDA amorphous ice transition. This is misleading since the melting of ice, which enhances the molecular amplitudes, is a phase transition even though the material undergoes a “dynamical transition” from solid to a liquid. The defining property of a “protein dynamic transition”, (glass transformation or percolation transition), is the structural continuity along the crossover. The molecular susceptibilities like specific heat show a discontinuity at the temperature, where the structural relaxation time crosses with the inherent time scale of the experiment**.** In the present case an apparent transition results from a pressure relaxation experiment. Fast cooling under pressure generates a non-equilibrium structure, which will progressively shift with T, as the solvent relaxes above 110 K. Ostermann et al. (ref, 7) explain, why no transition is expected with X-rays for slow cooling of protein crystals under ambient pressure conditions.