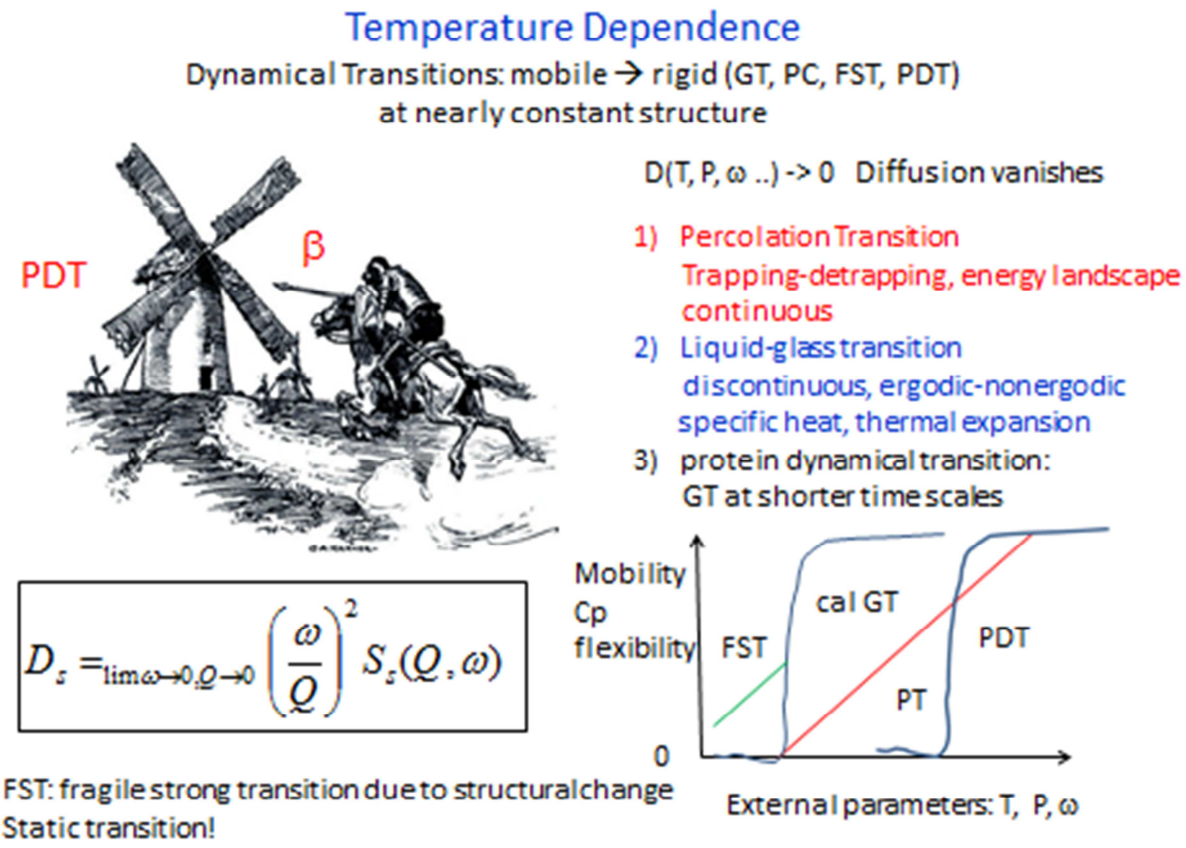
What is a Protein Dynamical Transition?

In Physics two kinds of dynamical transitions are discussed: The glass transition and the percolation transition. In both cases, the molecular mobility or diffusion vanishes below a particular temperature T_c. It is essential for a dynamical transition, that the structure remains fixed across T_c. A phase transition is not a DT although the mobility changes across a melting transition. The recently introduced Fragile-Strong Transition is not a dynamical transition, since it reflects a structural change. The glass transition is discontinuous, below T_g, the system appears solid. This occurs when the slow structural relaxation time crosses the time scale of the experiment, then the system falls out of equilibrium. This leads to a step in the specific heat, since slow degrees of freedom no longer contribute to the fluctuation spectrum.

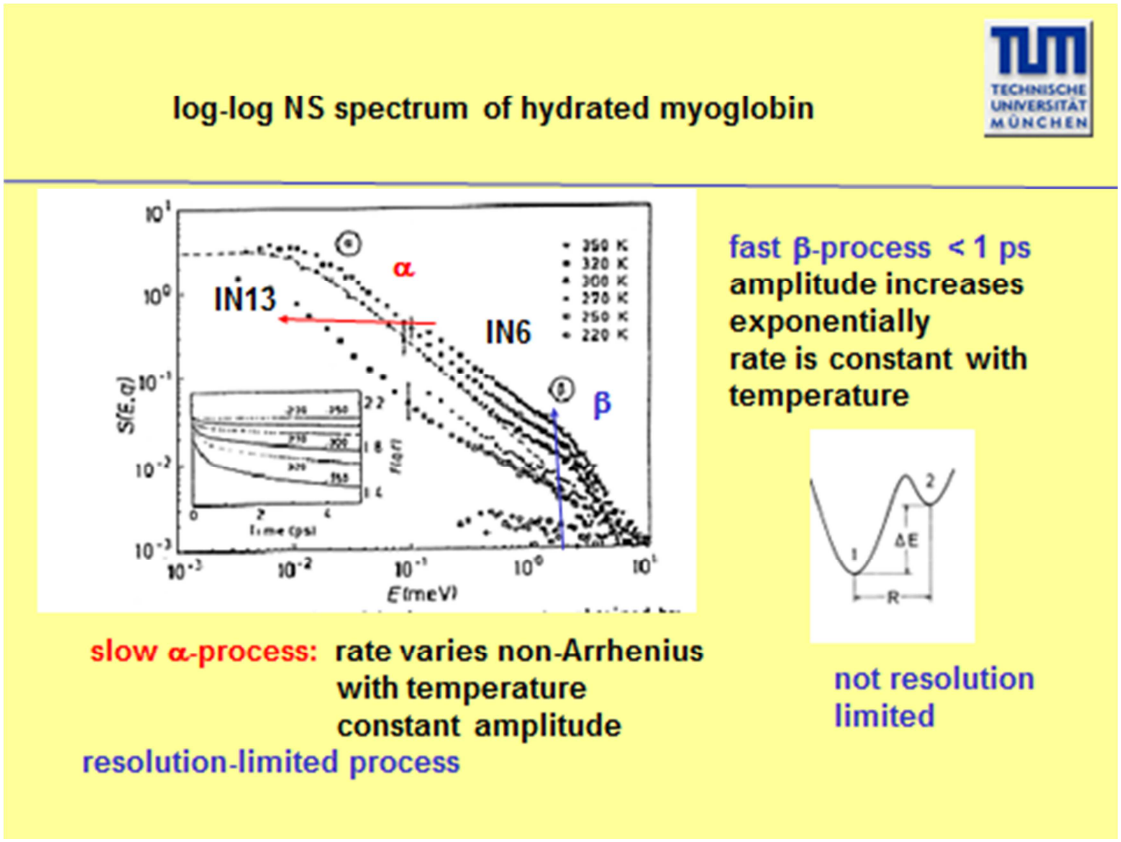
The percolation transition by contrast involves a continuous loss of mobility with temperature decrease, as it occurs for instance for trapping in energy wells.



(from my Les Houches Lecture 2013 above): That protein mobility goes to zero is consensus, but various types of transition are still discussed: FST: fragile-strong transition, calGT:calorimetric glass transition, PT: percolation transition, PDT: Protein Dynamical Transition.

The **Protein Dynamical Transition** (PDT) was defined in the context of the protein solvent glass transition observed with neutron scattering (W. Doster et al. Nature 1989, W. Doster et al. PRL (1990). With these two papers and the vibrational density of states paper by Cusack and Doster, Biophys. J. (1990) 58, 243 the Q and temperature dependent high frequency protein spectra were well defined by two types of fluctuations of the protein-solvent hydrogen bond network:

1) Fast local flucutations, opening and closing of hydrogen bonds on a picosecond time scale, which we called β- processes, with T-indpendent time scale, the motional amplitude increases with T: molecular rattling in cage of nearest neighbors.
2) The slow structural relaxation, which involves displacements of water molecules along the protein surface, which we called α-relaxation (see Comment for 1989).



If these processes are observed with a fixed frequency window method (elastic neutron scattering) as a function of the temperature, two transitions will emerge: In the elastic displacements $\langle \Delta x^2 \rangle$ near T_g (step in the thermal expansion, β) and the PDT (α) at T_D depending on the observation time (Doster, J. Noncryst. Sol (2011).

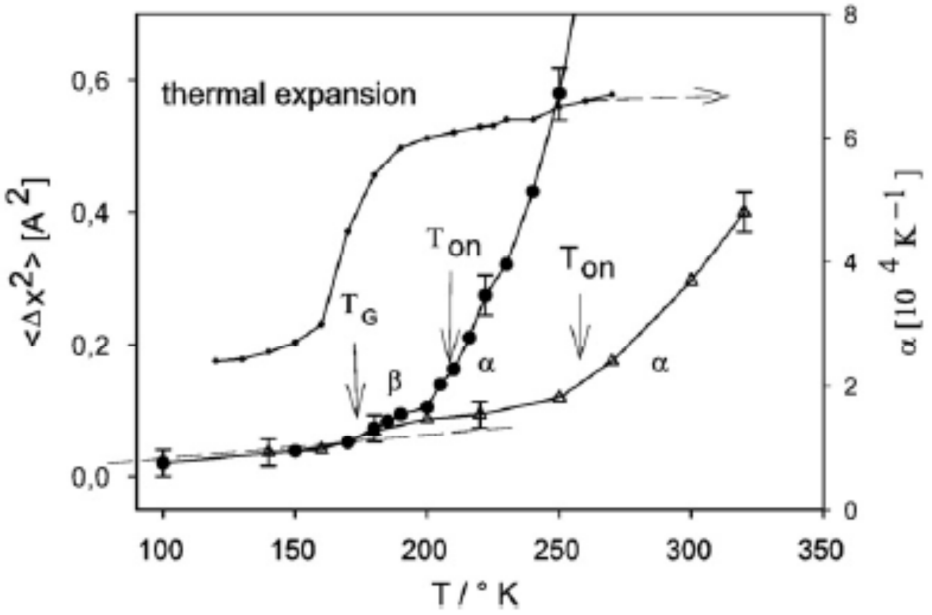


Fig. 7. Proton mean square displacements of H_2O adsorbed to C–PC at nominal time resolutions of 2 ns (full circles) and at 15 ps (open triangles, myoglobin). Dots: "Spectroscopic" thermal expansion coefficient (α) of water in hydrated myoglobin powder from the O–H stretching vibration [8,12]. The arrows locate the glass temperature T_g and the resolution-dependent onset temperatures T_{on} of the α-process. The resolution-independent onset of the fast beta-process is also marked. Dashed line: vibrational displacements.

The physical aspects of the PDT are well thus understood. In spite of a well documented literature an endless string of new interpretations of the PDT emerged (see Comments).

Recent summaries is given in:

W. Doster and M. Settles in Protein-Water Displacement Distributions, Bioch.Biophys.Acta (2005) 1749,172

W. Doster in Concepts and Misconceptions of the Protein Dynamical Transition, Eur.Bioph.J. (2008) 37, 591 (**).

W. Doster, The Protein-Solvent Glass Transition, Biochim. Biophys. Act.(Proteins, Proteomics (2010) 1084, 3-14

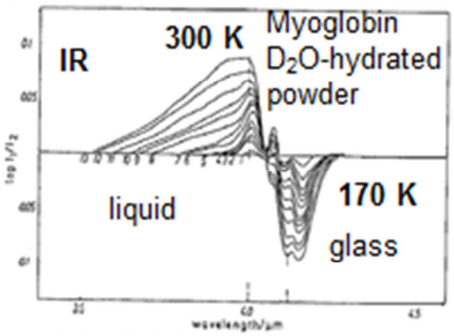
W. Doster in The Two Step Scenarion of the Protein Dynamical Transition, J. Noncr. Sol. (2011) 357, 622

W. Doster, H. Nakagawa and M.S. Appavou in Scaling Analysis of Biomolecular Motions by Elastic Incoherent Neutron Scattering, J.Chem. Phys. (2013) 139, 45105.

My pre-neutron scattering work with hydration water: IR and calorimetry:

Glass Transition of Protein Hydration Water was defined originally by IR O-D spectroscopy

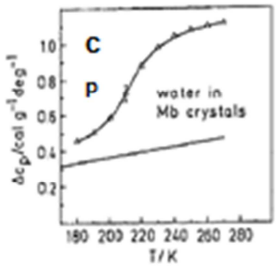
, W.D. Biophys.J. 50 (1986)



O-D stretching difference spectra: 100 - 300 K
liquid--> amorphous ice structure

Glass transition depends on time scale of experiment:
T_G(IR) < T_G(Möss) < T_G (diel)

100 s 140 ns 1 ns
(Doster BJ 1986)



Step of Specific heat of hydration water in myglobin crystals