

This unique letter still is the most profound publication of the field. It combines a wide-Q range elastic scattering analysis with a broad band spectral analysis. Dry and hydrated myoglobin and lysozyme were studied using time-of flight and backscattering spectroscopy at different resolutions covering the enormous temperature range of 300 degrees, 20 to 320 K. It set the basis of a model of protein dynamics of fast motions together with MD simulations:

- 1) The elastic scattering function  $S(Q)$  turns from a Gaussian displacement distribution at low temperatures (fig. 1) to a combination of an enhanced Gaussian and a non-Gaussian component. The non-Gaussian component emerging above 180 K was interpreted by rotational transitions of side chains, most methyl groups as we know today. The Gaussian enhancement above vibrational level by contrast occurs above 240 K and is observed only!! for hydrated proteins. This component was attributed to small scale motions coupled to hydration water displacements.
- 2) The second step was associated with the glass transition of hydration water and was thus called a “dynamical transition”. The dynamical transition thus occurs only with hydrated proteins! The first step, also present in dry proteins, was discussed as a pre-transition of fast local motions with T-dependent amplitude. The second step was interpreted as a time scale- or resolution- dependent feature. The calorimetric “glass transition” is associated with a 100 s time scale, while with neutron scattering one observes motions around 100 ps. We thus used the term “dynamical transition” for this short-time cross-over, which includes also the possibility of a percolation transition. The PDT was not just “dubbed” or pulled out of the pocket in contrast to the term “slaving”, which does not have a well-defined physical meaning.
- 3) The most important and novel achievement of this letter was the wide band and temperature protein spectra supporting the elastic analysis.  
 „Two spectral components with different shape and temperature dependence can be clearly recognized: a fast  $\beta$ -relaxation and a slower  $\alpha$ -process. The increase with temperature of the intensity of the broad line is consistent with local jumps between two states of energy asymmetry of 12 kJ/mol, Surprisingly however, the linewidth is temperature independent, correlation time 0.5 ps..... The line-width of the  $\alpha$ -relaxation by contrast broadens with increasing temperature. Below 240 K it is **not well resolved and contributes to elastic intensity....**”
- 4) Later work has shown, that the first step around 180 K was composed of two molecular processes: resolution-dependent methyl group rotations and fast amplitude controlled motions associated with the H-bond network.
- 5) In later work up to date only the elastic scattering analysis was adopted by the biologists as a simple tool to study protein dynamics: the shortcut to biology!