The dynamical transition of hydrated myoglobin observed by inelastic neutron scattering, W. Doster, S. Cusack and W. Petry Nature (1989)

This little letter still is a well cited, basic publication of the field. It combines a wide-Q range elastic scattering analysis with a broad band spectral analysis of hydrated myoglobin and lysozyme using together time-of flight and backscattering spectroscopy covering the enormous temperature range of 300 K, from 20 to 320 K.

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. These were attributed to small scale motions coupled to hydration water displacements.
2) From two component fits to the elastic scattering function low Q mean square displacements were derived. Two transitions were visible in the T-dependence (1) at 170-180 K and (2) at 240 K. The first transition was interpreted as an activation of side chain rotational transitions, modelled by an asymmetric two-state model, three state was also considered. 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 the relevant back-scattering time scale was 100 ps. We thus used the term "dynamical transition" for this 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 meaning.
3) ´The most important and novel achievement of this letter were the wide band and temperature dependent protein spectra supporting the elastic analysis. „Two spectral components with different shape and temperature dependence can be clearly recognized: a fast β-relaxation and a slower α-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 line-width is temperature independent, correlation time 0.5 ps….. The line-width of the α-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 (Doster, Settles BBA 2005), that the first step around 180 K is composed of two molecular processes: resolution-dependent methyl group rotations and fast amplitude controlled motions associated with the H-bond network near T_g. Thus the asymmetric two-state model applies only to the fast H-bond motions but not to methyl group rotation.

5) In later work mainly the elastic scattering analysis was adopted as a simple tool to study protein dynamics: the shortcut to biology!

Spectral analyis of hydrated myoglobin from Doster et al. Nature 1989.