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Zaccai neutron resilience and site-specific hydration dynamics in a globular proteins

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J. Smith et al. revive the old idea of J. Zaccai (Science,2000, fig. 2) that the average protein force constants k (N/m) can be deduced from the temperature slopes of hydrogen mean square displacements by elastic neutron scattering. The dynamical transition is supposed to reflect a change in protein elasticity:

k = k0 / (d<u^2>dT) see figure below:

a

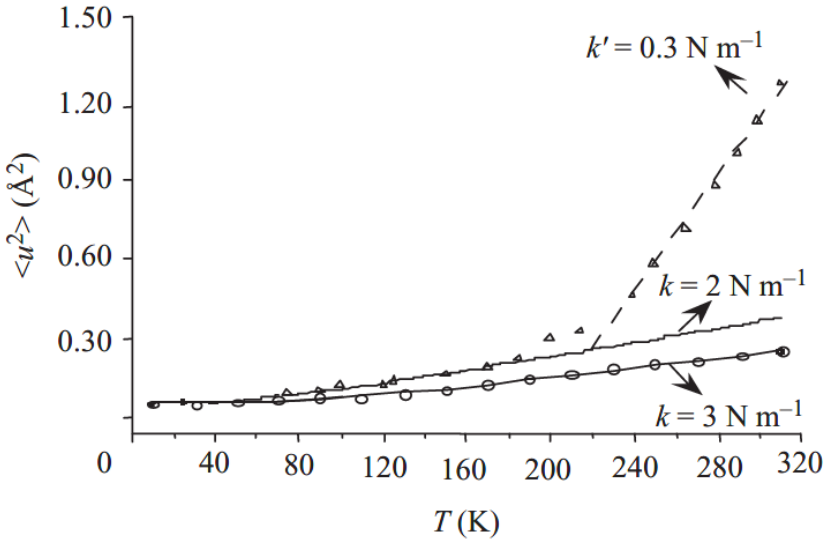
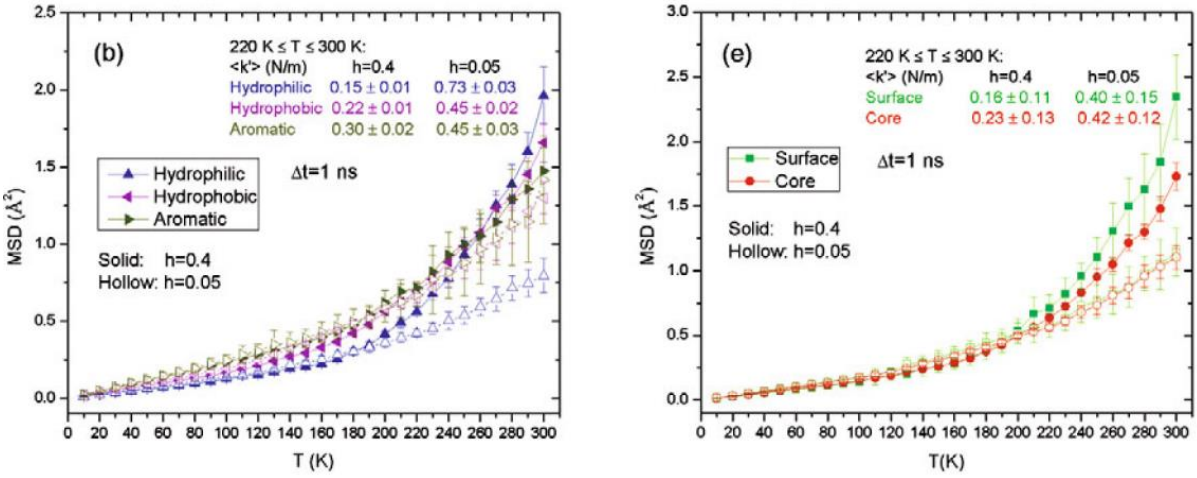


Figure 2. Quantifying internal forces in myoglobin. Mean square fluctuations ($\langle u^2 \rangle$) and effective force constants (k and k'), from neutron-scattering experiments in the ($\leqslant 1$ Å^2, 0.1 ns) length–time window. The data on hydrated myoglobin (triangles) and on myoglobin in a trehalose glass (circles) are from Doster *et al.* (1989) and Cordone *et al.* (1999), respectively. The force constant calculations are from Zaccai (2000).



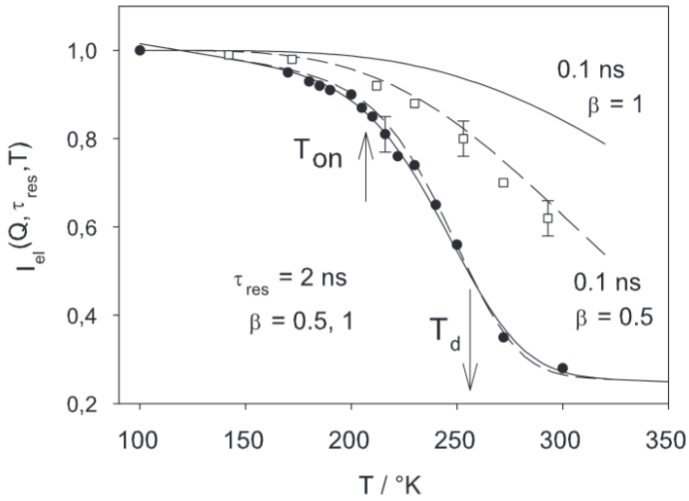
The figures reflect Smith's MSD simulations of P450 in 2013 including the 'resilence transition' and the respective force constants.

It is true that the low temperature harmonic or vibrational displacements display a slope, reflecting an effective force constant. In 2005 (Doster, Settles BBA) we have reproduced the experimental slope based on the measured vibrational density of states of myoglobin (Cusack, Doster, 1989). At high temperatures

the Zaccai force constant concept is however too simple: the resilence does not change at the transition temperature.

As we have pointed out in detail in 'Doster, Settles Protein Displacement Distributions, BBA 2005' and 'Concepts and misconceptisons of the protein dynamical transition', Doster, Eur.Bioph.J. 2008 the dynamical transition is not simply a resilence softening. It instead reflects molecular processes, whose correlation time starts to become resolved by the instrument: $\tau(mol) > \tau(res)$. In a special sense, if probed on a time scale faster than $\tau(res)$, the protein appears to be harder, no softening can occur by structural relaxation. On slow times $\tau >> \tau(res)$, the structure can flow. This resembles a liquid to glass transition: Any liquid behaves as a glass on a short enough time scale.

The figure below shows the elastic intensity of CPC hydration water at two different resolutions 0.1 and 2ns versus the temperature taken from Doster et al. JCP(2013). The dynamical transition obviously depends on the instrumental resolution. T_{on} is the onset temperature, while T_d localizes the time scale identity of $\tau(res) = \tau(water)$ and the exponent β.



The question of protein force constants, derived from elastic neutron scattering has been picked up recently in

Nakagawa et al. Biophys.J. (2021) 120, 5408, Dynamics of natively disordered proteins in solution and force constants.