EPJ Web of Conferences **272,** 01009 (2022) https://doi.org/10.1051/epjconf/202227201009
QENS/WINS 2022

Intracellular molecular dynamics studied by neutron scattering

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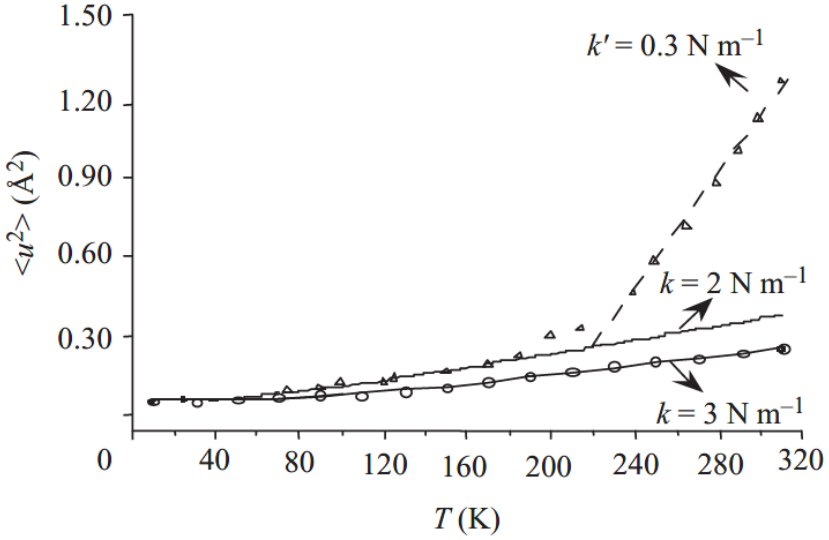

Figure 2. Quantifying internal forces in myoglobin. Mean square fluctuations ($<u^2>$) and effective force constants (k and k'), from neutron-scattering experiments in the ($\leqslant 1$ Å^2, 0.1 ns) length–time window. The data on hydrated myoglobin (triangles) and on myoglobin in a trehalose glass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

Comment: The figure above shows a famous bio-neutron scattering result, first published by J. Zaccai in Science (2000). Since then it was republished many times. In 2013 it won the Walter Hälg neutron price. The version above is taken from Smith et al. Its message did not change in 22 years: We are looking at the hydrogen mean square displacements of hydrated myoglobin (triangles), compared to those of myoglobin embedded in a sucrose glass (circles). The hydrated case shows a 'protein dynamical transition' at 200 K together with J. Zaccai's interpretation as a structural softening in the force constants 'k'. In contrast, the vitrified protein does not show a softening transition. This seems quite plausible, it is not correct however for two reasons: (1) The static protein force constants do not change at the transition, it is a dynamic effect and (2) even in the vitrified state one can observe a transition in the temperature slope of <u2>. To see that, one has to employ a perdeuterated glassy matrix, otherwise the elastic signal of the protonated glass overwhelms the protein dynamics of surviving methyl rotational motions (Doster, EBJ 2008).