Science & Technology Facilities Council
ISIS

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Thermal motion in the multi-subunit protein apoferritin as probed by high energy resolution neutron spectroscopy

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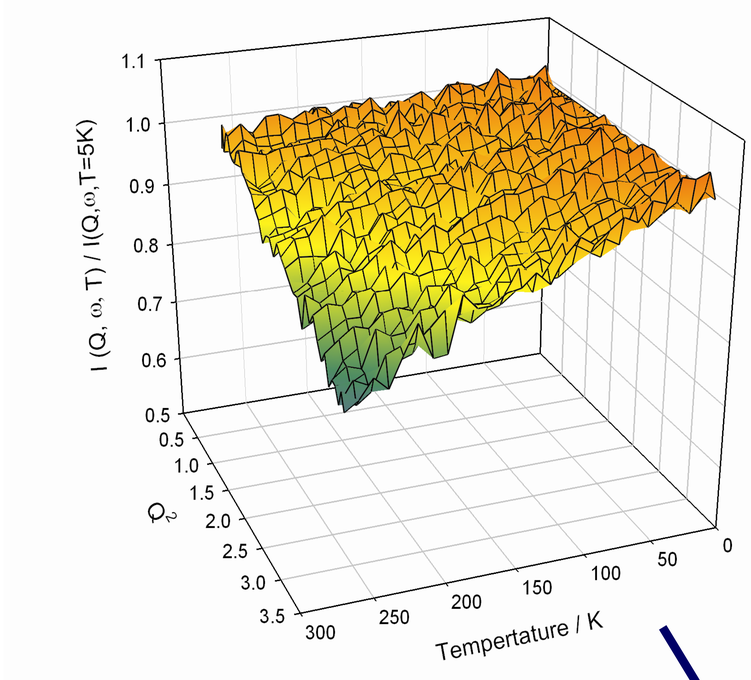
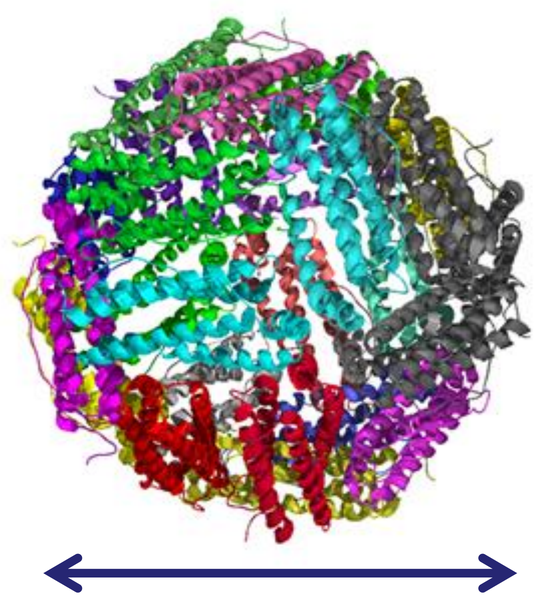
$\Gamma_{res,\ fwhm}$ = 24.5 - 4.0 μeV
t_{max} = 0.07 - 0.30 ns
ΔE = ± 400 - ± 150 μeV



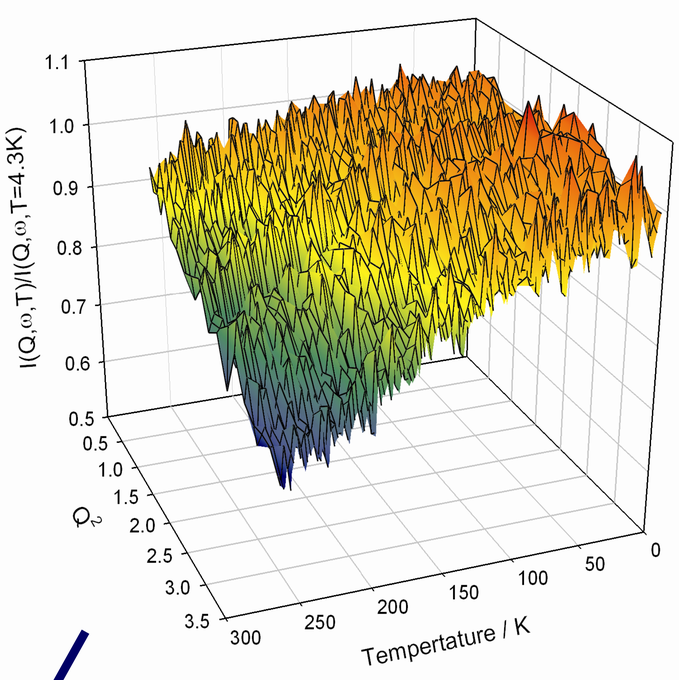


120 Å

24 peptide chain, hollow, quaternary structure of apoferritin
internal diameter = 80 Å

IN16

$\Gamma_{res,\ fwhm}$ = 0.9 μeV
t_{max} = 2 ns
ΔE = ± 14 μeV



simultaneous fit of elastic scattering data to CH_3 jump rotation model [1]

$$S(Q,\omega\approx 0,T)=\exp\left(\frac{-Q^2<r^2>}{3}\right)\times\left((1-p_m+(p_m\times A_o(Q)))+\frac{2}{\pi}[1-(1-p_m+(p_m\times A_o(Q)))]\times\sum g_i\arctan\left(\frac{\Gamma_{res}}{\Gamma}\right)\right)$$

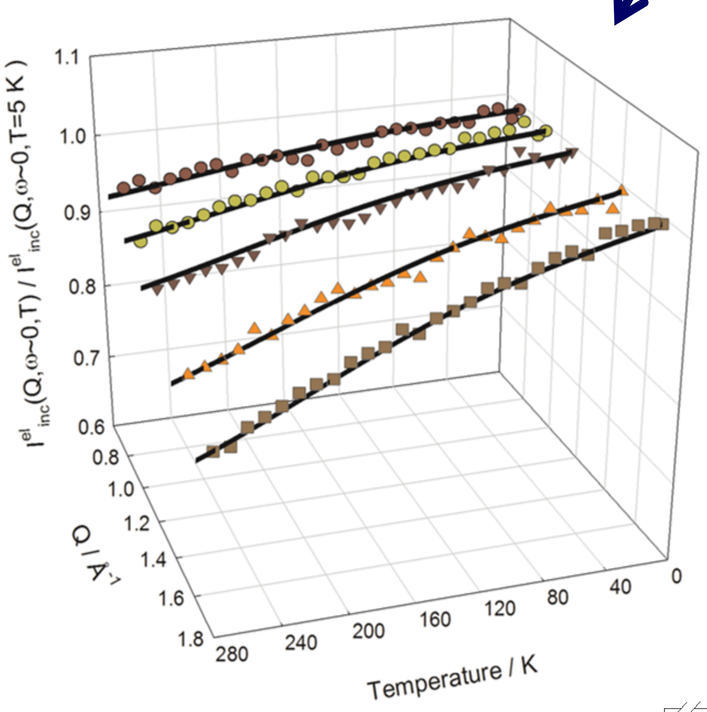
with the theoretical assumptions

$$A_o(Q)=\frac{1}{3}\left[1+2\,j_o(\sqrt{3}Qa)\right]$$

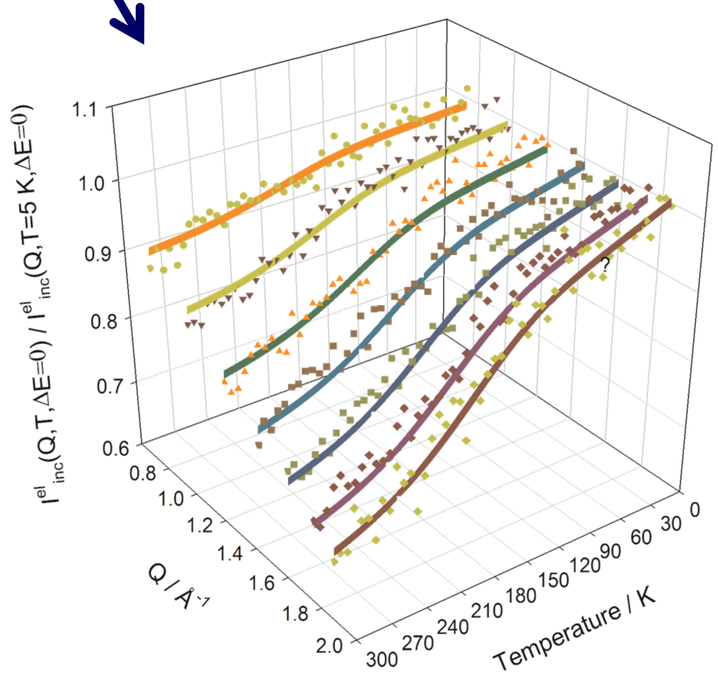
and

$$\Gamma=\Gamma_o\exp\left(-\frac{E_a}{RT}\right)$$

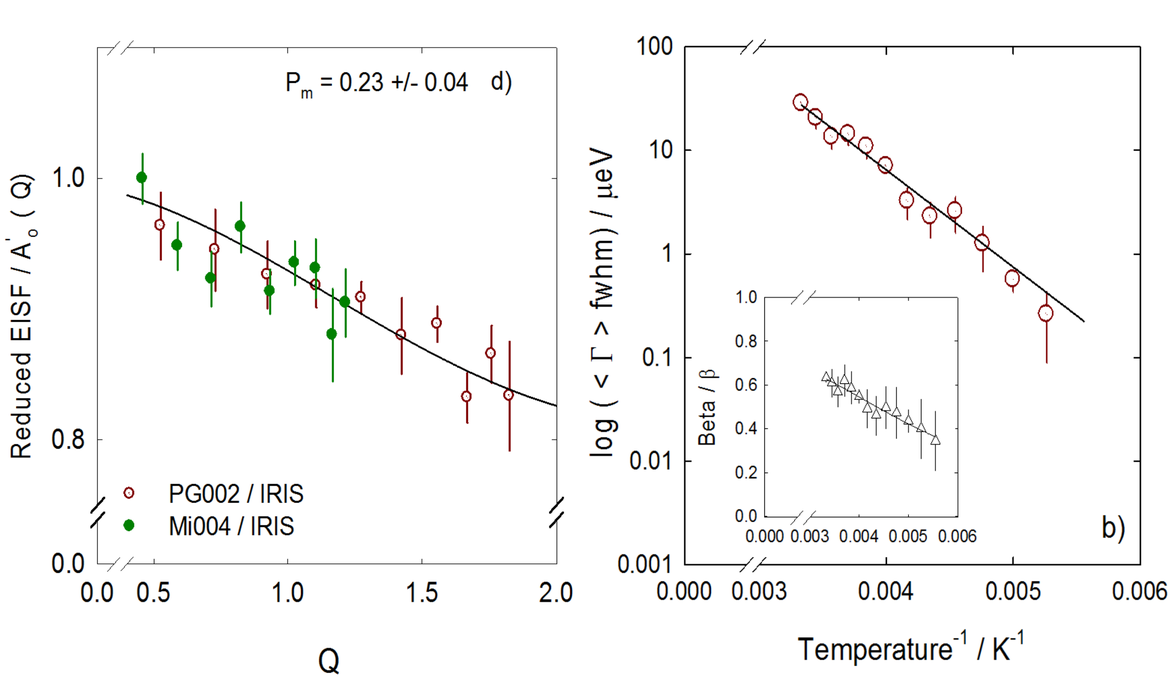
being validated experimentally...



from: M.T.F Telling *et al*
J Phys Chem B, 2008



from : M.T.F Telling *et al*
Soft Matter, 2011



Lyophilised apoferritin, *above T~100K and in the ps-ns time regime,* ***exhibits a single dynamic response driven by methyl groups alone***

No contribution is observed from protons associated with non-CH_3 species

A distribution of CH_3 activation energies is obtained in line with the environmental heterogeneity

[1] V. Arrighi and J.S. Higgins, Journal of the Chemical Society-Faraday Transactions 1997