An Instrument Concept for Dynamics of Complex (Bio-) System from Elastic Scattering

There is no ad-hoc technique to measure complex systems (e.g., bio-molecules). Benedicto developed Resolution Elastic Neutron Scattering (RENS) and with DjaJ Kreelley developed an instrument dedicated to RENS.

RENS is a model-free way to extract $T_{relax}$ and the agreement with QENS is excellent in this case shown below. Lysozyme hydration H$_2$O $\rightarrow$ QENS is RENS independent on a model.

$S_R(\omega, 0, T_{ess}) = \int dt I(\omega, t) R(t, T_{ess})$

Measured Elastic Scattering System Dynamics Resolution Function

$S_R(\omega, 0, \Delta \omega) \rightarrow$ "system" domain $T_{ess} \geq T_c$ $S_R = S_{system}$

$S_R(\omega, 0, \Delta \omega) \rightarrow$ "resonance" domain $T_{ess} \approx T_c$

$S_R(\omega, 0, \Delta \omega) \rightarrow$ "instrument" domain $T_{ess} \ll T_c$ $S_R = R$

$\lambda = \frac{d \sin \theta}{\Delta \omega} = \frac{\Delta \omega}{\tan \theta} + \frac{d}{d}$

Varying Monochromator-sample distance and Monochromator curvature yields different instrumental energy resolutions.

McStas simulations

$\Delta \omega = 19 \text{ meV}$ $\Delta \omega = 24 \text{ meV}$

ChemistrySimulations $S_R(t, T_{ess}) = \int I(\omega, t) R(t, T_{ess}) d\omega$

$S_R(t, T_{ess}) = \frac{I(t, T_{ess}) R(t, T_{ess})}{I(t, T) R(t, T_{ess})}$

ESS vs. QENS $\Delta \omega / T_c = 5\%$

But... Inefficient! Since it requires multiple backscattering spectrometers.

But what if we had an instrument with measurable resolution...? Elastic Scattering Spectrometer (ESS)

Constant Wavelength Setup (cw source) Focusing Monochromator Incident White Beam

Detectors Sample Beam Stop Crystal Analyzers

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Proteins in water (as measured with $\Delta \omega = 0.3 \text{ meV}$ on 11M B)

Dry Protein $\rightarrow$ "Rink" shifts to lower T $\rightarrow$ H$_2$O dynamics faster than protein.