

50 Years of Neutron Backscattering Spectroscopy



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Investigation of Molecular Dynamics: Exceed the Gaussian Approximation

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We investigate the dynamics of bio-molecules with the help of incoherent neutron scattering. For elastic data sets the mean square displacement (MSD) as a function of temperature is extracted which may depend strongly on the instrument resolution, Q -range and analysis method employed. This makes it difficult to compare quantitatively data sets from different bio-molecules and experimental data with MD simulations.

Our goal is to find out how quantitatively MD simulations can reproduce the trends of experimental data over a range of different systems and instruments and under many different conditions like temperature, pressure, hydration, pH/pD or crowding. In addition, it is important to figure out to what extent such trends may depend on sample preparation, data reduction and data analysis.

Generally, from elastic data the MSD is extracted based on the Gaussian approximation with Q values normally not exceeding 2\AA^{-1} . Here, we present data on a larger momentum transfer range - up to $Q=5\text{\AA}^{-1}$ as measured on the neutron backscattering spectrometer IN13 at the Institut Laue Langevin (ILL) - and investigate the accuracy of different models which have been proposed lately. This could point to the extraction of more information from elastic data sets.

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