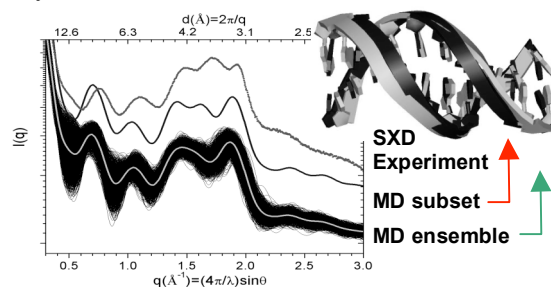


X-ray Diffraction “Fingerprints” of Biomolecular Structure and Dynamics in Solution. D.M. Tiede, X. Zuo, A. J. Goshe, Chemistry Div., Argonne National Laboratory, Argonne, IL, 60439.

Advances in synchrotron X-ray scattering techniques offer new opportunities for characterization of biomolecular structure and dynamics in non-crystalline media that build upon crystallographic, NMR, and molecular dynamics (MD) databases, but are applied to conditions relevant to in-situ function. Advances include extension to the high-angle domain where measurements can be routinely made to a spatial resolution of 1 Å, and the development of coordinate-based analyses that allows scattering data to be analyzed in terms of detailed coordinate models for structure and dynamics. Solution X-ray diffraction (SXD) “fingerprint” patterns provide a 1D summary of 3D structure. Peak positions and linewidths are found to provide direct measures of structure and configurational dispersion, respectively. We have found that experimental SXD patterns can be used as benchmarks to discriminate between crystallographic, NMR, and MD models for solution state protein and DNA structures, and to “refine” coordinate models to fit solution state data. Comparisons to MD simulation for A-tract (polyA-polyT) DNA reveal shortcomings in the underlying force fields that skew simulated ensembles toward B-form conformers.



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