THE POTENTIAL OF CSAXS (CORRELATED SAXS) FOR OBSERVING SUPERCOILS IN RANDOMLY ORIENTED ENSEMBLES OF DNA FRAGMENTS

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The advent of X-ray free electron lasers (xFEL's) makes possible the measurement of angular correlations in azimuthal deviations from the angular mean measured in SAXS profiles[1]. We will present simulations of correlated SAXS (CSAXS) from DNA fragments and show that they exhibit a characteristic azimuthal symmetry dependence which measures the relative width to persistence length ratio. We use a weakly jointed chain model to simulate the size-dependence of this ratio as a function of the size of DNA fragments. We show that CSAXS can measure the degree of supercoiling in DNA plasmids. We discuss the possibility of using this technique to monitor the degree of supercoiling of bacterial chromosomes *in vivo*.

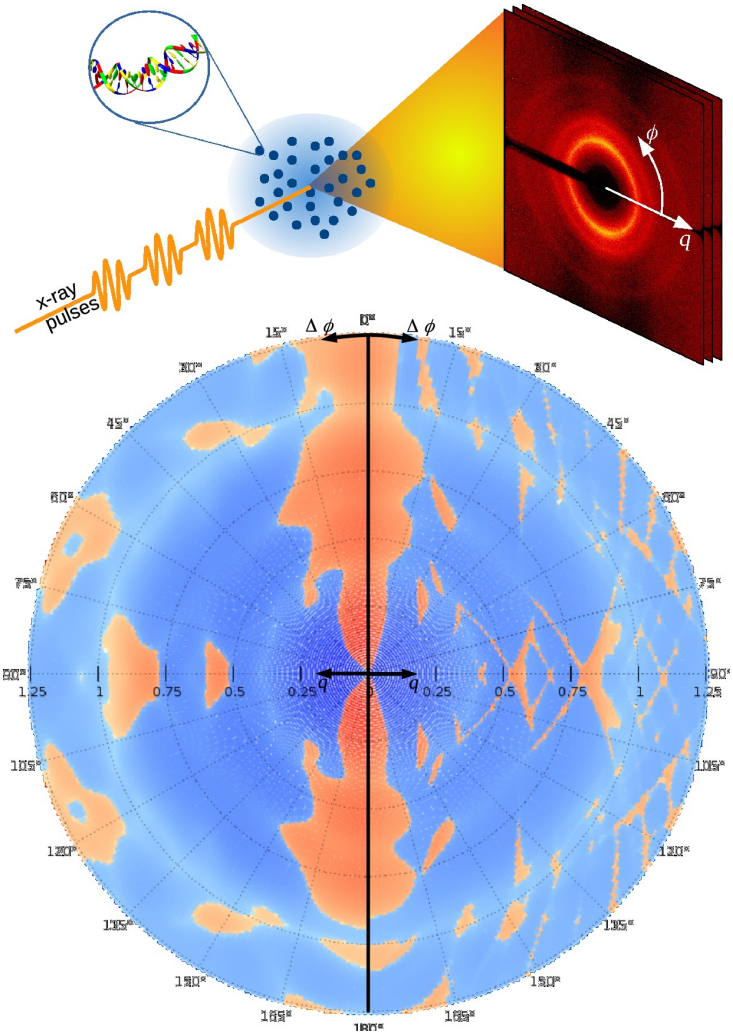

Figure 1: Simulated angular autocorrelations of solution X-ray scattering images. Left:17bp DNA, right: 134bp DNA.

The average over many angular correlations of scattering measurements at low q contains information of the thermodynamic persistence length of the DNA molecules and their degree of supercoiling. At higher q the correlation patterns relate to the internal molecular structure.

A simple test supports that uncorrelated scattering events from other randomly placed molecules tend to obscure in the correlation average. Therefore and because of the inherent three-dimensional information, CSAXS has the potential to become an advantageous technique to traditional solution SAXS..

References

[1] D. Mendez *et al*, Phil. Trans. Roy. Soc. 369 (2014) 20130315.

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