Angular Correlation Small Angle Scattering of Gold Rods in Aqueous Solution

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It has long been suggested to carry out high-resolution imaging of non-periodic objects at 3rd and 4th generation light sources by the method of single-particle diffractive imaging. In that method, diffraction patterns of particles are acquired one at a time in various orientations.[1] Recent theoretical work by Saldin et al. has proposed a method by which the diffraction from multiple, randomly oriented identical objects can be deconvolved and the scattered intensity of a single object can be reconstructed utilizing angular spatial correlations (Figure 1).[2] Once the single particle scattering intensity is recovered, traditional phase retrieval algorithms can be used to reconstruct the real space electron density. The ability to reconstruct numerous identical particles are important for the ease of sample delivery, scattered intensity and damage thresholds of radiation sensitive materials, especially biological samples. Previous experimental work has imaged identical stationary particles on membranes as a proof of principle experiment and the angular correlations were determined.[2] These particles lie in a common scattering plane, and are only randomly distributed about a single rotational axis. The most direct application is for membrane proteins embedded in their native membrane where there is inherent alignment along one axis.[3] For wider applicability, however, this algorithm must be shown to work on flowing or injected samples, where many biological samples can be imaged in their native environment. The challenge is to image the particles with enough scattered intensity at a short enough timescales that rotational diffusion will not strongly affect the scattered intensities. Flowing or injected particles will also not be imaged in the same scattering plane and the algorithms must be sufficiently robust to work for particles randomly oriented about multiple rotational axis.

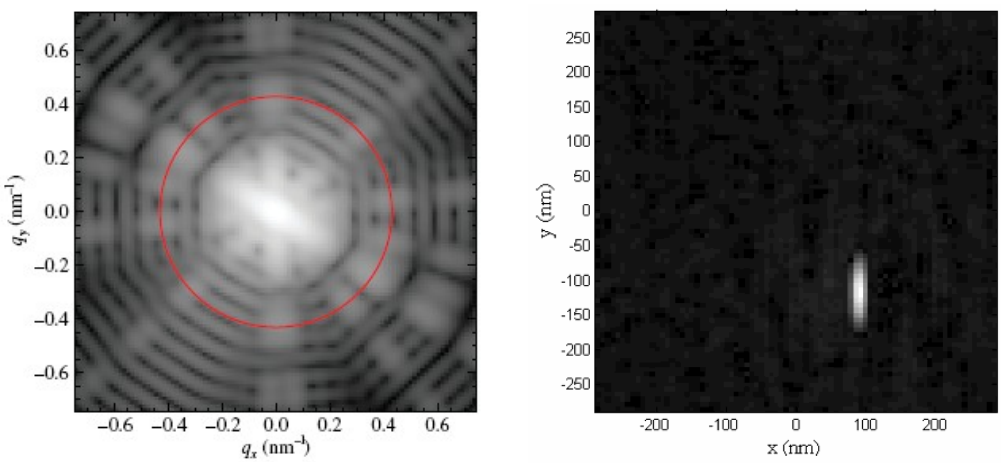

Figure 1: (a) Simulated diffraction pattern of 10 randomly oriented rods and (b) the real space charge density of a single rod whose single particle diffraction intensity is reconstructed from 100 simulated patterns such as (a)

An unfocused, coherent 8keV beam at the Coherence Applications Beamline, P10, at Petra III, was used to obtain the Small Angle Scattering (SAXS) of identical gold microrods of size 200x1000nm. The rods were suspended in a surfactant and water environment at a concentration of approximately $1x10^8$ particles/ml, corresponding to an average of 10 particles in the illumination volume of the

beam. The particles were imaged in a stationary state with only rotational and translational diffusion, and also flowing. SAXS images of multiple microcrystals were taken at various acquisition times. The acquisition time determines the scattering strength of the sample and will affect the imaging resolution as rotational and translational diffusion will blur out the scattering from single particles. SAXS patterns at acquisition times of 0.5 sec, 0.3 sec and 0.1 sec are shown in figure 2. The strength of the scattering signal decreases at shorter acquisition times but at longer times, SAXS signal from individual stationary microrods are no longer distinguishable.

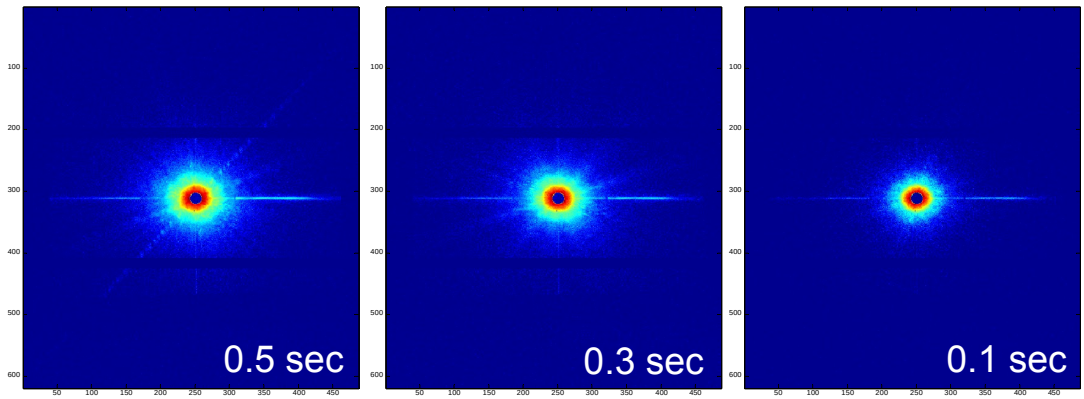

Figure 2: SAXS patterns of 200nm x 1000nm gold rods in aqueous solution taken at various acquisition times.

This represents the first experimental work in obtaining SAXS diffraction of identical objects in random rotations about 2 axis for the purpose of angular correlation reconstruction. The parameters needed for successful reconstruction, namely the particle concentration and the acquisition time will be determined from the analysis of the acquired patterns. Future work will involve flowing high aspect ratio samples to maximize alignment along one axis to aid the angular correlation algorithm reconstruction of a single particle diffraction pattern from multiple particle diffraction. Ongoing theoretical work and analysis of the reconstructability of multiple particle diffraction of particles randomly oriented not only in the scattering plane but also along orthogonal axis will widen the applicability of this technique to objects which are not inherently aligned.

References

[1] H.N. Chapman, Nature Materials **8**, 299–301 (2009).
[2] D. Saldin *et al* , New J. Phys. **12**, 035014 (2010).
[3] D. Saldin *et al* , Phys Rev B **81**, 174105 (2010).