Atomic Jumps by Atomistic-Scale Photon Correlation Spectroscopy

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Collecting series of diffuse scattering patterns with coherent X-rays aXPCS (atomic-scale X-ray Photon Correlation Spectroscopy) method has become a very powerful technique to probe atomic motion in crystalline and amorphous materials. The resulting "motion picture" provides information on the dynamics dependent not only on the temperature but also on the flux of the incident beam, which could be seen as a great opportunity to indirectly probe physical properties of materials like e.g. bonding features.
High brilliance coherent X-ray beams are available only on few exclusive synchrotron sources with a very limited access guided by an elaborate proposal process. In order to give students an opportunity to sample an aXPCS experiment and evaluation in our lab, we prepared a simple experiment with a laser light to measure and evaluate nanoparticles motion in liquids, widely known as Brownian diffusion. Theoretical basis of this process, referred to as a PCS or dynamic light scattering (DLS), is very similar to the principles of coherent X-rays research and evaluation, thus enabling a smooth entrance into synchrotron scattering experiments.
In DLS experiment coherent laser light scattered by a particle suspension forms a random diffraction or speckle pattern fluctuating in time as particles move due to Brownian diffusion [1]. For the current workshop different sets of fluctuation intensities measured in our laboratory with a single photon-counting detector will be provided to participants for subsequent computer analysis. A short theoretical introduction will be sufficient as a basis for understanding of the method. Software for calculation of the autocorrelation function will be allocated on desktop computers or can be built by a competent programmer in a few hours. An essential element of the workshop is a graphical presentation of the data and fit lines, which can be easily handled by a gnuplot. Gnuplot [2] is a portable command-line driven, freely distributed graphing utility for many computer platforms. Fig. 1 shows exemplary illustration of raw data from a detector and estimated dynamics of milk in water suspension.

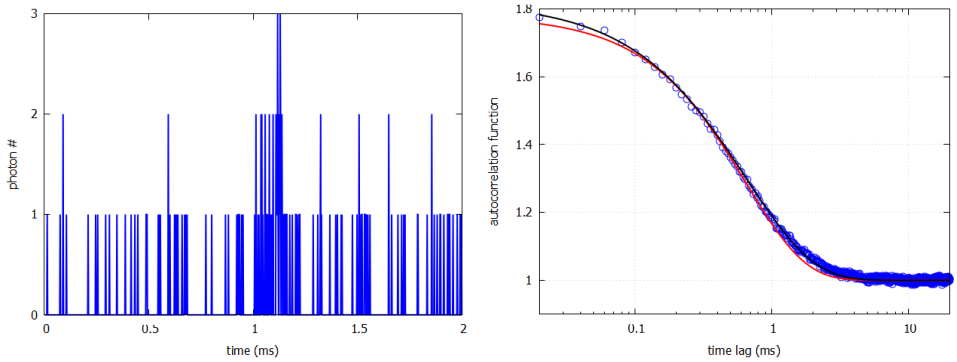

Figure 1: Left: sketch of photon bunches scattered by fat particles in milk. Right: autocorrelation function calculated from light scattering on milk as a function of time lag between scattering events. Red line is a simple exponential fit, black line is fitted with a normal distribution of particle diameters.

[1] P.N. Pusey, Neutrons, X-rays and Light: Scattering Methods Applied to Soft Condensed Matter, chapter 9, North-Holland, 2002.
[2] http://www.gnuplot.info/