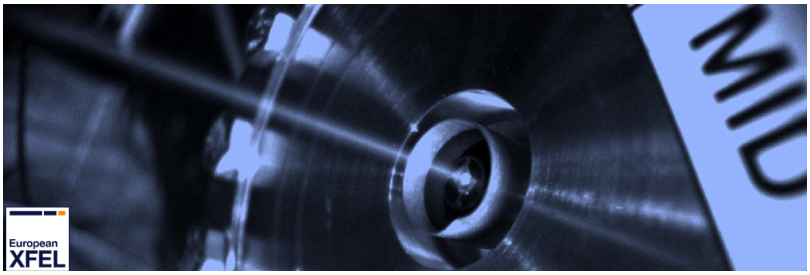

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Ultrafast atomic pair distribution function analysis

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The atomic pair distribution function method is growing in popularity as an approach for studying local structure in nanomaterials, amorphous materials, moleculare materials and liquids, as well as a growing interest in the study of local symmetry breaking in bulk crystals. It is a direct measure of the local structure in the vicinity of an atom. As such, it is a very interesting representation of the structure in the context of time resolved measurements, becuase if the local bonding state or coordination of an atom is changed through photoexcitation, the PDF gives a direct measure of that change, and how the change propagates out in time from the location where it occured.
Despite this, to date there has been very little work in measuring ultrafast PDFs (ufPDFs). The reasons are technological rather than scientific. First, the resolution of the PDF in real space is directly determined by the measured range in momentum, Q. To get quantitatively reliable PDF high Qmax values of greater than 20 inv. angstroms are required, and this requires good fluxes of short wavelength x-rays (> 20 keV) to be used. Second, it is required to measure this wide range of reciprocal space quantitatively with low backgrounds and linear detector response. These limitations are now being addressed with latest generation large area 2D detectors and the developing of hard-x-ray free electron lasers.
I will describe the PDF and how it could, in principle, be used in an ultrafast time resolved context. I will then describe our recent attempt to obtain moderate resolution, quantitatively reliable, PDFs in an ultrafast PDF experiment at LCLS at SLAC. The initial results are very promising, which opens the door to much more extensive quantitative time resolved local structural studies.

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