High-quality ultra-fast total scattering and pair distribution function data using an X-ray free electron laser

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Total scattering and pair distribution function (PDF) methods are essential for resolving local atomic structure in disordered, nanocrystalline, and non-equilibrium materials [1]. However, conventional synchrotron measurements are fundamentally limited in time resolution, restricting access to the femtosecond structural dynamics that underpin many functional processes. In this talk, I will present the first demonstration of quantitatively reliable total scattering and PDF data obtained from single ~30 fs X-ray free-electron laser (XFEL) pulses [Fig. 1a] [2]. Using the High Energy Density (HED) instrument at the European XFEL [3], we achieved normalized structure factors over a wide momentum-transfer range (0.35–16.6 $Å^{-1}$), enabling real-space PDFs with near-synchrotron quality [Fig. 1b]. The performance of the approach is validated across a broad range of systems, including crystalline and nanocrystalline powders, amorphous solids, liquids, and atomically precise clusters in solution [2]. Crucially, these data are compatible with established analysis workflows, including Rietveld refinement, small-box PDF modelling, and Debye scattering analysis. This work establishes XFELs as viable sources for quantitative total scattering and opens the door to true femtosecond-resolved 'molecular movies' of disorder, nucleation, and non-equilibrium structural transformations.

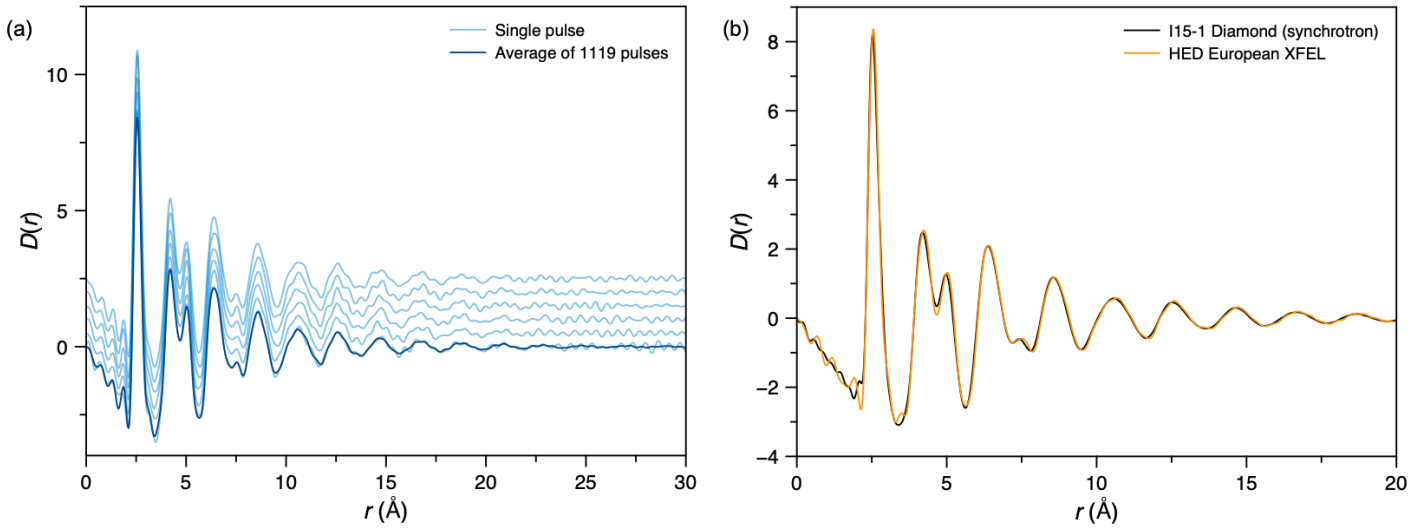


Figure 1. *(a) Average (black) and single ~30 fs pulse (blue) PDFs obtained from a metallic glass. (b) Comparison between PDFs obtained from XFEL and synchrotron radiation.*

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