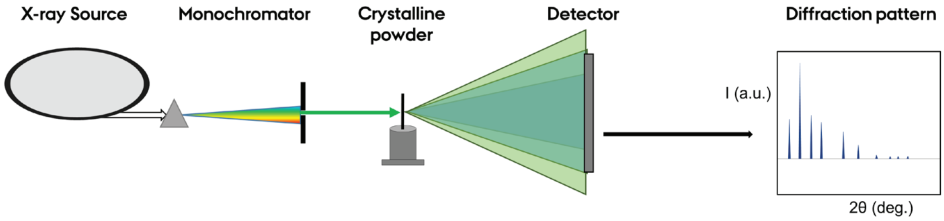
COMBINING X-RAY TOTAL SCATTERING AND CONVENTIONAL X-RAY DIFFRACTION

Functional materials are crucial to modern technology. In this LINX project, researchers from Aarhus University develop state-of-the-art methods for analysing the structure of functional materials.

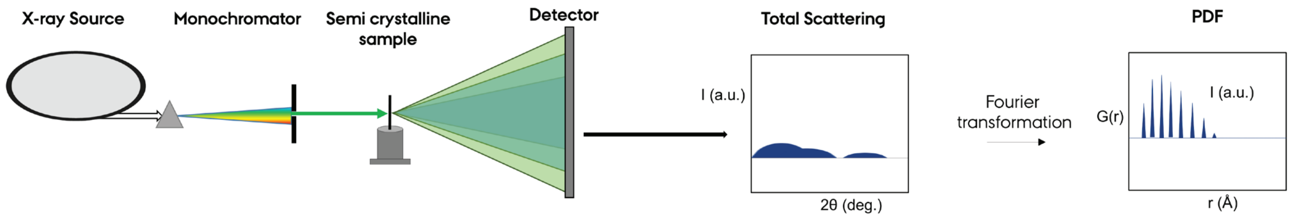
Rietveld analysis of diffraction data has long been the standard method in materials science to obtain ratios of mixed crystalline phases. This method, however, fails to reveal potential non-crystalline phases as well as local deviations from the long-range average crystal structure. By using a wider detection range to collect so-called "total scattering" data, it is however possible to quantify every interatomic distance in a material, regardless of the crystallinity. Researchers from Aarhus University combine X-ray total scattering and conventional X-ray diffraction techniques to study functional materials, where small defects and deviations from the average crystal structure can be decisive for the properties, as well as multiphase systems, containing both crystalline and amorphous phases at the same time.

POWDER X-RAY DIFFRACTION



Synchrotron X-ray diffraction on a crystalline powder sample. The long-range average crystal structure is analyzed from the Bragg peaks while any diffuse scattering is described as a background contribution. Hence, local defects and deviations from the average crystal structure as well as potential amorphous phases are not revealed.

TOTAL X-RAY SCATTERING



Synchrotron X-ray total scattering from a "real world" semi crystalline sample. Mathematically, the total scattering data are Fourier transformed into the Pair Distribution Function (PDF), which contains information on the distribution of atomic pairs within a sample.

In the LINX project, researchers at leading Danish universities collaborate with scientists in industry to solve industry relevant problems using advanced neutron and X-ray techniques. The group of Bo Brummerstedt Iversen at Aarhus University contributes with their expertise in materials crystallography and diffraction techniques. The LINX Project has received funding from Innovation Fund Denmark (IFD).

READ MORE
linxproject.dk

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LINX Linking Industry to Neutrons and X-rays

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