Poster Presentation

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PDF Analysis on a Laboratory System: Adapting the Experiment to the Material

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The increased interest in recent years regarding the properties and applications of nanomaterials has also created the need to characterize the structures of these materials. However, due to the lack of long-range atomic ordering, the structures of nanostructured and amorphous materials are not accessible by conventional diffraction methods used to study crystalline materials. One of the most promising techniques to study nanostructures using X-ray diffraction is by using the total scattering (Bragg peaks and diffuse scattering) from the samples and the pair distribution function (PDF) analysis. The pair distribution function provides the probability of finding atoms separated by a certain distance. This function is not direction-dependent; it only looks at the absolute value of the distance between the nearest neighbors, the next nearest neighbors and so on. The method can therefore also be used to analyze non-crystalline materials. From experimental point of view a typical PDF analysis requires the use of intense high-energy X-ray radiation ($E \geq 20$ KeV) and a wide 2θ range. After the initial feasibility studies regarding the use of standard laboratory diffraction equipment for PDF analysis [1-3] this application has been further developed to achieve improved data quality and to extend the range of materials, environmental conditions and geometrical configurations that can be used for PDF experiments. Studies performed on different nanocrystalline and amorphous materials of scientific and technological interest, including organic substances, oxides, metallic alloys, etc. have demonstrated that PDF analysis with a laboratory diffractometer can be a valuable tool for structural characterization of nanomaterials. This contribution presents several examples of laboratory PDF studies, in which the experimental conditions have been successfully adapted to match the specific requirements of materials under investigation.

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