Application of Pair Distribution Function Analysis on a laboratory diffractometer in the temperature range 80 – 1400 K

Narygina O. [1*], Sommariva M. [1], Reiss C.A. [1], Gateshki M. [1], Fransen M.J.[1], Quinn J.[2], Pein A.[3]

[1]PANalytical B.V., Almelo, The Netherlands

[2] PANalytical Inc, Westborough, MA, United States

[3]Anton Paar GmbH, Graz, Austria

The total X-ray scattering (Bragg peaks and diffuse scattering) technique and the pair distribution function (PDF) analysis [1] is a powerful method to study the structural properties of different materials. It can be used to analyze both crystalline and non-crystalline materials, as opposed to the conventional X-ray diffraction methods, which rely on the presence of a long-range order and are therefore restricted to the study of crystalline materials.

From experimental point of view, a typical PDF analysis requires the use of intense high-energy X-ray radiation ($E \geq 15$ KeV) and a wide 2θ range. After the initial feasibility studies regarding the use of standard laboratory diffraction equipment for PDF analysis [2-4] 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 crystalline, 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 wide range of materials [2-6].

Recent progress in detector technology (e.g. GaliPIX^{3D} detector with CdTe chip[5]) have enabled the application area of laboratory PDF to be extended towards *in situ* analysis. The high efficiency and high resolution of GaliPIX^{3D} detector provide excellent data quality for total scattering measurements on a laboratory instrument reducing the data collection time to just few hours. Combining GaliPIX^{3D} detector with various non-ambient attachments allows *in situ* PDF experiments in the temperature range from 80 to 1400 K.

This contribution presents several examples of laboratory *in situ* PDF studies of crystalline and nano-crystalline materials, in which the experimental conditions have been successfully adapted to match the specific requirements of the materials under investigation.

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