

# Poster Presentations

**[MS27-P04] Ambient and non-ambient temperature PDF studies on a laboratory instrument.**

Céleste. A. Reiss<sup>a</sup>, MilenGateshki<sup>a</sup>, Marco Sommariva<sup>a</sup>,

**Keywords:** pair distribution function (PDF), high-energy in-house X-rays diffractometers, nanocrystalline materials

<sup>a</sup>PANalytical B.V., Almelo, The Netherlands.

E-mail: Celeste.Reiss@PANalytical.com

Nanoscaled materials have been a subject of increased interest during the last decade due to their specific properties. For this kind of materials, 'standard' inhouse X-ray powder diffraction measurements give broad Bragg-like features and pronounced diffuse scattering contribution. Well crystallized materials on the other hand give sharp Bragg peaks which can be used for structure determination and refinement of these materials. While synchrotron and neutron sources remain the preferred choice for Pair Distribution Function (PDF) analysis, there is clearly an increasing need for a PDF solution based on in-house diffraction equipment. Such a solution, though limited, will benefit areas where quick feedback about the materials properties is important and will allow the routine application of PDF analysis for materials characterization in university laboratories as well as industrial R&D departments [1]. Recently we have extended our ambient high-energy diffraction measurements to non-ambient temperatures. This presentation describes the latest developments of laboratory (non)-ambient X-ray equipment for PDF analysis and discusses some results obtained with such equipment. One of the examples is the (non)-ambient pair distribution function studies on ammonia borane,  $\text{NH}_3\text{BH}_3$ , a material which received considerable attention recently as a potential hydrogen storage material. Other examples are  $\text{C}_{60}$  and  $\text{H}_2\text{O}$  both measured at room and low temperature.

[1] Reiss, C.A., Kharchenko, A., Gateski, M. 2012, *Z. Kristallogr.*, **227**, 257.