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Total Scattering: The Structural Characterization Tool For The 21st Century. Th. Proffen, Los Alamos National Laboratory, LANSCE-12, Mailstop H805, Los Alamos, NM 87545.

Structural characterization is mainly based on the measurement of Bragg intensities and yields the average structure of the crystalline material. However, this approach ignores any defects or local structural deviations that manifest themselves as diffuse scattering. It also fails in case of materials that are badly crystalline such as many nanomaterials or not crystalline at all, such as glasses. Nevertheless, in all these cases a total scattering experiment using all the information, yields local and medium range structural information [1].

Here we present different applications of this technique including data taken on the new high resolution neutron powder diffractometer NPDF located at the Lujan Neutron Scattering Center at Los Alamos National Laboratory. This instrument is design for total scattering studies using the Pair DIstribution Function (PDF) approach. The instruments high resolution in reciprocal space one to obtain PDFs up to distances of $r=100-200\text{\AA}$. This hope is to attract many new users to use total scattering as a tool to fully characterize their materials structurally.

¹Th. Proffen, S.J.L. Billinge, T. Egami and D. Louca, Z. Krist. 218, 132-143 (2003).