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Structural Characterization of Complex Materials using Pair Distribution Function Analysis. Thomas Proffen, *Lujan Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, NM, USA.*
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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 disordered materials, badly crystalline such as many nano-materials, or not crystalline at all, such as glasses. In some cases crystalline and amorphous phases coexist making the traditional crystallographic structure refinement difficult or incomplete. The total scattering pattern, however, contains structural information over all length scales [1] and can be used to obtain a complete structural picture of complex materials. Suddenly one has access to a new parameter, the real-space range of the refinement and structures can be analyzed as function of length scale straight forwardly. A classic example is LaMnO_3 , here the average structure shows that the MnO_6 octahedra in become regular when the material is heated above 1000K, but total scattering measurement show [2], the octahedra stay regular up to the highest temperatures. The reason is the fact that the MnO_6 octahedra stay distorted, and only the cooperative orientation of the Mn-O long bonds disappears. Since the atomic Pair Distribution Function (PDF) extracted from total scattering data contains structural information as function of length scale r , one can study the transition from the local to the average structure. In this presentation an overview of experimental advances in neutron and x-ray total scattering measurements as well as the current state-of-the-art in modeling of disordered materials will be presented. Examples include local disorder in exotic oxides, nano-particles and their ligand structure as well as complex systems such as 'green' geopolymer concrete.

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[2] X. Qiu, Th. Proffen, J.F. Mitchell and S.J.L. Billinge, *Phys. Rev. Lett.* 94, 177203 (2005).

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Disorder phenomena in Prussian Blue analogues. Dmitry Chernyshov^a, Alexei Bosak^b. ^a*Swiss-Norwegian Beam Lines at European Synchrotron Radiation Facility, France.* ^b*European Synchrotron Radiation Facility, France.*
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Prussian Blue (PB), probably the first coordination compound ever synthesized by mankind, together with its metal substituted analogues attract nowadays growing interest due to photo-magnetism, magnetic pole inversion, photo-chromism, light induced structural phase transformations. All these switching phenomena start as a local process, like charge transfer or a change of the spin state of metal ions, then coherently propagate through the bulk to form a new macroscopic state on a scale of hundreds of unit cells. At the scale from few to few tens of the unit cells a propagation of

the local process would be strongly affected by the correlated structural disorder. Physical properties at this mesoscopic scale are not yet understood due to the lack of structural information on disorder.

We use diffuse scattering of synchrotron radiation to characterize structural disorder in a manganese-based Prussian Blue analogue. Full 3D mapping of diffuse intensity has been performed and parameterized by a correlated compositional distribution of $[\text{Mn}(\text{CN})_6]^{3-}$ units and $(\text{H}_2\text{O})_6$ clusters. We describe the observed correlated disorder by an analytical 3D autocorrelation function which is further used to generate extended clusters with required correlation properties. Structural correlations we observed might be generic for the entire family of disordered Prussian Blue analogues and should be used for realistic modeling of switching phenomena.

Keywords: Diffuse scattering, Prussian Blue, synchrotron radiation

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Defective Coordination Polymers. Norberto Masciocchi^a, Simona Galli,^a Angelo Maspero,^a Antonietta Guagliardi,^{a,b} Antonio Cervellino^c.
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Coordination polymers constitute a large portion of the covalent materials nowadays studied for their functional properties, ranging from molecular recognition, gas storage and separation, catalysis, magnetic and optical properties. [1] Thus, the knowledge of their structures is a fundamental issue in the design and preparation of new materials for tailored optimized species. When possible, the conventional single-crystal diffraction technique is the method of choice, unless only powdered, microcrystalline samples are available. Our recent work has demonstrated that *ab-initio* powder diffraction methods is a powerful tool for retrieving the crystal and molecular structures of such materials, [2] addressing the existence of constitutional isomers, polymorphs, oligomeric vs. polymeric forms, etc. However, we have often found that these materials, not affording single-crystals of suitable quality, also show "poor" powder diffraction traces, with anisotropically broadened peaks or very broad diffraction features, making their (physically meaningful) modeling troublesome. Therefore, selected examples from our recent work, using also total scattering methods (by the Debye Function approach [3]) will be presented, highlighting the structural features that conventional methods (Rietveld-like) alone could not disclose.

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