s12.m34.o1 **From Crystalline to Amorphous: Total Scattering Used as Universal Local Structural Probe**. Th. Proffen, *Lujan Neutron Scattering Center, LANL, MS H805, Los Alamos, NM 87545, USA. E-mail: tproffen@lanl.gov*

Keywords: Pair Distribution Function; Powder Diffraction; Disorder

Knowledge of the atomic scale structure is an important step towards understanding and possibly predicting the properties of materials. Scattering is a powerful tool to unravel the atomic structure of materials. In case of crystalline materials, conventional structure determination is based on the analysis of the intensities and positions of Bragg reflections. It should be noted, that the study of Bragg reflections only reveals the long range *average* structure of the material. However, many real materials of technological importance are disordered and their properties are often governed by this disorder. In this case the diffraction pattern will show diffuse scattering which contains information about two-body interactions or the local atomic arrangements to a deeper understanding of the properties of the material. One method to reveal the local structure is the analysis of the atomic pair distribution function (PDF). The PDF is obtained via Fourier Transform of a properly normalized total powder diffraction pattern.

Thinking as a crystallographer, amorphous materials can be considered the most disordered case, showing no Bragg reflections at all. In fact, the PDF method has long been used to obtain local structural information from glasses or liquids. More recently the PDF technique has been extended to study disordered crystalline materials, and it becomes apparent that total scattering (Bragg- and diffuse scattering) is an ideal tool to probe the short- and even medium range atomic structure of materials in general. Using high-energy X-rays or neutrons, the resolution in real space of ~0.1Å can be achieved. Recently the neutron powder diffractometer NPDF at the Lujan Neutron Scattering Center at Los Alamos National Laboratory became available to the user community interested in high-resolution PDF studies.

s12.m34.o2 **Using Evolutionary Algorithms for the Investigation of Disordered Materials**. Thomas Weber, *Lab. of Crystallography, ETH Zurich, Switzerland. E-mail: thomas.weber@mat.ethz.ch*

Keywords: Disorder; Evolutionary Algorithms; Diffuse Scattering

In the last decade the availability of new experimental tools like third generation synchrotron sources and powerful area detectors was accompanied by a significant increase of computing power. This combination opened the possibility of simulating disordered structures based on high quality diffuse scattering data. The introduction of Monte Carlo (MC) methods as modelling techniques was an important step, because it allowed describing even complicated disorder phenomena by only a few parameters. Initially, MC simulations were used as a qualitative tool only, *i.e.* simulated diffraction patterns were visually compared to the experimental diffraction patterns. Later, least-squares methods were used to optimize the underlying model parameters and to minimize the differences between experimental and simulated intensities [1]. An intrinsic problem of least-squares methods is, however, that they require starting values close to the final values before this technique can successfully be used. Otherwise, this procedure is prone to get stuck in a local minimum. On the other hand, searching for good start values by trial-and-error is a very time consuming procedure, which also requires some expertise. A major part of this work can be left to the computer, if the parameter space is searched by evolutionary algorithms [2]. In this contribution the principles of evolutionary techniques and their application to crystallographic disorder problems are outlined. Based on several examples, potential and practical problems of this technique will be discussed.

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[2] Weber, T. & Burgi, H. B.: Determination and refinement of disordered crystal structures using evolutionary algorithms in combination with Monte Carlo methods. *Acta Cryst*. A**58**(2002) 526-540.