

# Whole Pair Distribution Function Modelling: the Bridging of Bragg and Debye Scattering Theories

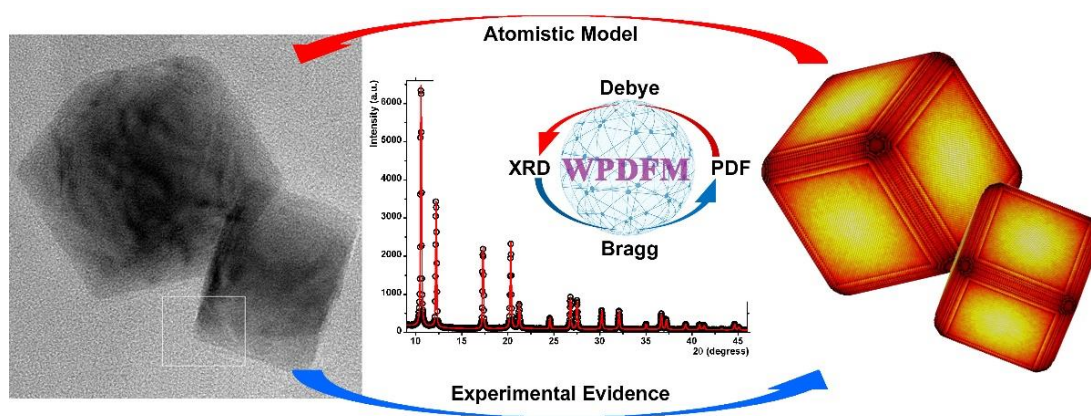
Alberto Leonardi

Institute for Multiscale Simulation, IZNF, Friedrich-Alexander University Erlangen-Nürnberg, Erlangen, 91058, Germany  
Department of Earth and Atmospheric Sciences, Indiana University, Bloomington, Indiana 47405, U.S.A.

alberto.leonardi@fau.de

The microstructure design of materials requires an atomic-level understanding of mechanisms underlying structure-dependent properties. The analysis of either the traditional diffraction profile or the pair distribution function (PDF) gives access to the long- or short-range information. Any variation of structural and microstructural features over the whole sample affects Bragg's peaks as well as the underneath diffuse scattering. Accuracy of characterization relies, therefore, on the reliability of the analysis methods and employed models. Bragg's methods investigate the diffraction peaks in the intensity plot as distinct pieces of information.<sup>1</sup> This idea hits its limitation when dealing with disorder scenarios that do not compare well on such a peak-by-peak basis. Debye methods tackled directly the scattering from a disordered phase.<sup>2</sup> However, the structure information is averaged in the short-range, and statistical reliability and computing efficiency are sacrificed.

Here we introduce the whole pair distribution function modeling method, which directly targets the intermediate regime disorder in materials. We use Bragg's models to ease the computation of a whole PDF and then model powder scattering data *via* the Debye scattering equation (DSE). Bragg's models allow the efficient solution of the dispersion of crystallite's properties in a powder sample with statistical reliability, while the PDF yields the flexibility of the DSE. The whole PDF is decomposed into the independent directional components and the number of atom pairs separated by a given distance is statistically estimated.<sup>3</sup> This allows us to avoid the need for an atomistic model of the material sample and the need for the computation of the billions of pair distances. Besides the results being in perfect agreement with the explicit solution of the DSE, our method allows us to take advantage of the strengths and different sensitivity of the Bragg theory.



1. Scardi, P. & Leoni, M. *Acta Crystallogr. A* **58**, 190–200 (2002).
2. Debye, P. *Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen* **27**, 70–76 (1915).
3. Leonardi, A., Leoni, M. & Scardi, P. *J. Appl. Crystallogr.* **46**, 63–75 (2013).