Utilizing the Debye Equation in Nanomaterial Line Profile Analysis

K. Beyerlein[1,2*], R.L. Snyder[1], and P. Scardi[2]
1. Georgia Institute of Technology - Department of Materials Science & Engineering - 771 Ferst Dr. - Atlanta, GA, 30332 - USA
2. University of Trento - Department of Materials Engineering and Industrial Technology - via Mesiano 77 - 38100 Trento, TN - Italy
[*] Contact author - e-mail: ken.beyerlein@mse.gatech.edu

The design of materials at the nanometer scale has allowed scientists to rethink how to engineer materials with a desired set of properties. The structure of these materials governs many of their properties and assembly mechanisms. X-ray Powder Diffraction is an important tool to measure the local atomic arrangement, and is indispensable to pushing forward the understanding of these materials. With respect to other complementary techniques like Transmission Electron Microscopy, powder diffraction is statistically sound and relatively inexpensive, that can directly be transferred to commercial applications and quality control.

A developing approach to Line Profile Analysis is to model a measured pattern using the Debye Equation to calculate the powder diffraction pattern from a volume of scatterers. This allows for matching of the measured diffraction pattern with a representative atomistic model, which contains a wealth of information, is very robust, and versatile. The drawback is that as the size of the system increases, the number of necessary calculations increases as the volume squared. However, modern computing power allows this technique to be employed to simulate the pattern from nanosized materials on a reasonable timescale. This approach is not yet well known, therefore a brief tutorial on its use and possible applications will be presented. The use of the Debye Equation for quantitative characterization of a microstructure requires its implementation into a non-linear least squares routine. A program of this type has been developed based on the Levenberg-Marquardt algorithm. Its ability to arrive at the correct set of microstructure parameters describing the size, strain, and defects present in a system of nanoparticles will be showcased as well.