

**MS38-1-1 Error Bounds of Pair Distribution Function Analysis in Characterization of Thermal Disorder in Nanocrystals**  
**#MS38-1-1**

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**Abstract**

Pair distribution function (PDF) analysis is a novel tool that is becoming popular in structural characterization of nanocrystals from their diffraction signature. However, there are no established accuracy bounds of the recovered structural parameters from PDF analysis [1]. In this work, we present a self-consistent computational workflow to address this question. By performing PDF analysis on simulated diffraction profiles of realistic gold nanocrystals at various temperatures, we compare temperature induced structural parameters such as lattice parameters and atomic displacements from PDF analysis to those from direct atomistic calculations [2,3] at finite temperatures.

**References**

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