MS39 Crystallography at the nanoscale

MS39-04
Evaluating the Accuracy of Rietveld Analysis for Diffraction Data from Nanocrystalline Powders
H. Hekmatjou [1], H. Ozturk [1]

[1]Ozyegin University - Istanbul (Turkey)

Abstract
Powder X ray diffraction is a widely used method to evaluate the structural properties of nanocrystalline powders. However, direct application of crystallographic solution algorithms are not compatible with the true structural characteristics of such materials [1, 2]. In this study, we present a computational workflow based on first-principle atomistic formulations of diffraction data to evaluate the performance of Rietveld refinement analysis in quantifying average atomic displacements of monodispersed and ideally random powders of gold nanocrystals. We show that the accuracy of the extracted thermal displacements of atoms (isotropic displacement parameters and microstrains) depend strongly on the average sizes of the investigated nanocrystals.

References
[1] Xiong, S.; Ozturk, H.; Lee, S.-Y.; Mooney, P. M.; Noyan, I. C., The nanodiffraction problem. Journal of Applied Crystallography 2018, 51 (4), 1102-1115.
[2] Xiong, S.; Lee, S.-Y.; Noyan, I. C., Average and local strain fields in nanocrystals. Journal of Applied Crystallography 2019, 52 (2), 262-273.