Nanocrystalline Powder Diffraction Analysis

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This presentation will outline the basic theory of diffraction from nanocrystalline powder samples and highlight several implicit assumptions within currently employed formalisms which grow weaker with decreasing particle size. For this study we used rigorous computer modeling [1,2] to analyze powder diffraction and were able to link the intensity within each pixel of a 2-D detector to the specific grains from which this intensity originates. Our simulations showed that the sampling rules and diffraction grain statistics must be modified when one analyzes the diffraction pattern from nanocrystalline powder samples. These issues required modifications in fundamental concepts like "reflection multiplicity" and the "Lorentz factor".

In addition to modifying statistics and selection rules for powder diffraction, the decrease in sample size also caused changes in the angular dependence of the scattering power of individual crystallites. This caused a particle-size-dependent error in lattice parameters, obtained from single-peak, multi-peak or whole-pattern refinement approaches, which is important for particle sizes below 15 nm[3]. For the smallest particles the error could be large.

The presentation will conclude with some suggestions for testing powder pattern data for the presence of these issues.

References

[1] "*Correlating Sampling and Intensity Statistics In Nanoparticle Diffraction Experiments*", Journal of Applied Crystallography, **48**, 2015.

2] "*Expected Values and Variances Of Bragg Peak Intensities Measured In a Nanocrystalline Powder Diffraction Experiment*", Journal of Applied Crystallography, **50**, 2017.

[3] "*The Nanodiffraction Problem*", Journal of Applied Crystallography, **51**, 2018.

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