MS38-2-1 Investigation of Pair Distribution Function Method on Structural Analysis of Nanocrystalline Powders #MS38-2-1

A. Baloochiyan [1], H. Ozturk [1]
[1]Ozyegin University - Istanbul (Turkey)

Abstract
This self-consistent computational work presents the minimum errors of structural parameters (e.g. lattice parameters, crystalline size, atomic displacement parameters) expected from Pair Distribution Function (PDF) analysis of nanocrystalline gold powders. Recently, PDF analysis has gained momentum in naocrystalline powder characterization by X-rays, however, current literature does not contain expected error bounds of the resulting structural parameters. For an accurate interpretation of X-ray diffraction data, the error bounds must be analyzed. We aim to address this problem in three steps: 1. Simulation of ideal powderdiffraction experiments with the use of the Debye scattering equation, 2. PDF analysis of the diffraction data, and 3. Determination of the errors from PDF analysis by comparing them with real-space analysis of spherical gold nanocrystals with sizes of 30 nm and smaller. Our results demonstrate that even for the ideal nanocrystals in ideal diffraction conditions, the extracted structural parameters from PDF analysis diverge from their true values. These deviations are dependent on the average size of the nanocrystals and the wavelengths of the illuminating X-rays. In diffraction analyses of nanocrystalline powders, lower X-ray energies and smaller crystal sizes are prone to greater uncertainties in extracted structural parameters.

References
1. Prasad N, Karhikeyan B. Tunable bandgap and blue emission of ZnS nanoparticles induced by controlled S vacancies. Journal of Applied Physics 2019; 125: 085702. < 10.1063/1.5083656>.
2. Tran N, Zhao W, Carlson F, Davidson JH, Stein A. Metal Nanoparticle-Carbon Matrix Composites with Tunable Melting Temperature as Phase-Change Materials for Thermal Energy Storage. ACS Applied Nano Materials 2018; 1: 1894-1903. <10.1021/acsanm.8b00290>.
3. Ingham B. X-ray scattering characterisation of nanoparticles. Crystallography Reviews 2015; 21(4): 229-303. < 10.1080/0889311X.2015.1024114>.
4. Kang S-JL, Park J-H, Ko S-Y, Lee H-Y. Solid-State Conversion of Single Crystals: he Principle and the State-of-the-Art. Journal of the American Ceramic Society 2015; 98(2): 347-360. < 10.1111/jace.13420>.
5. Neder RB, Proffen T. Exact and fast calculation of the X-ray pair distribution function. Journal of Applied Crystallography 2020; 53: 710-721. <10.1107/S1600576720004616 >.
6. Rietveld HM. A profile refinement method for nuclear and magnetic structures. Journal of Applied Crystallography 1969; 2: 65-71. < 10.1107/S0021889869006558>.
7. Juhas P, Farrow C, Yang X, Knox K, Billinge S. Complex modelling: a strategy and software program for combining multiple information sources to solve ill posed structure and nanostructure inverse problems. Acta Crystallographica 2015; A71: 562-568. < 10.1107/S2053273315014473>.
8. Petkov V, Bedford N, Knecht MR, Weir MG, Crooks RM, Tang W, Henkelman G, Frenkel A. Periodicity and atomic ordering in nanosized particles of crystals. Nanoscale 2008; 112 (24):8907-8911. < 10.1021/jp801195c>.
9. Popa NC, Balzar D. Size-broadening anisotropy in whole powder pattern fitting. Application to zinc oxide and interpretation of the apparent crystallites in terms of physical models. Journal of Applied Crystallography 2008; 41: 617:627. < 10.1107/S0021889808012223>.
10. Bugaev AL, Guda AA, Lomachenko KA, Shapovalov VV, Soldatov AV, Lazzarini A et al. Core-Shell Structure of Palladium Hydride Nanoparticles Revealed by Combined X-ray Absorption Spectroscopy and X-day Diffraction. The Journal of Physical Chemistry C 2017; 121: 18202-18213. < 10.1021/acs.jpcc.7b04152>.
11. Xiong S, Öztürk H, Lee S-Y, Mooney P, Noyan IC, The nanodiffraction problem. Journal of Applied Crystallography 2018; 51:1102-1115. < 10.1107/S1600576718007719>.
12. Toby BH, Egami T. Accuracy of pair distribution function analysis applied to crystalline and non-crystalline materials. Acta Crystallographica 1992; A48: 336-346.
< 10.1107/S0108767391011327>.
13. Farrow CL, Billinge SJL. Relationship between the atomic pair distribution function and small-angle scattering: implications for modelling of nanoparticles. Acta Crystallographica 2009; 65(3): 232-239. < 10.1107/S0108767309009714 >.
14. Plimpton S. Fast Parallel Algorithms for Short-Range Molecular Dynamics. Journal of Computational Physics 1995; 117 (1): 1-19. < 10.1006/jcph.1995.1039>.
15. Sheng HW, Kramer MJ, Cadien A, Fujita T, Chen MW. Highly optimized embedded-atom-method potentials for fourteen fcc metals. Physical Review B, 2011; 83 (13): 134118. < 10.1103/PhysRevB.83.134118>.
16. Öztürk H., Yan H., Hill JP, Noyan IC. Sampling statistics of diffraction from nanoparticle powder aggregates. Journal of Applied Crystallography 2014; 47: 1016-1025. < 10.1107/S1600576714008528>.
17. Debye P. Zerstreuung von Röntgenstrahlen. Annalen der Physik 1915; 46: 809-823. < 10.1002/andp.19153510606>.
18. Warren BE, X-ray Diffraction. New York, NY, USA: Courier Corporation, 2012. ISBN: 978-0486663173

19. Juhas P, Davis T, Farrow CL, Billinge SJL. PDFgetX3: A rapid and highly automatable program for processing powder diffraction data into total scattering pair distribution functions. Journal of Applied Crystallography 2013; 46: 560-566. < 10.1107/S0021889813005190>.
20. Trueblood KN, Bürgi HB, Burzlaff H, Dunitz JD, Gramaccioli CM, Schulz HH, Shmueli U, Abrahams SC. Atomic Displacement Parameter Nomenclature. Report of a Subcommittee on Atomic Displacement Parameter Nomenclature. Acta Crystallographica 1996; A52: 770-781. < 10.1107/S0108767396005697>.
21. Dippel A-C, Roelsgaard M, Boettger U, Schneller T, Gutowski O, Ruett U. Local atomic structure of thin and ultrathin films via rapid high-energy X-ray total scattering at grazing incidence. IUCrJ 2019; 6: 290-298. < 10.1107/S2052252519000514 >.
22. Gilbert B. Finite size effects on the real-space pair distribution function of nanoparticles. Journal of Applied Crystallography 2008; 41: 554-562. < 10.1107/S0021889808007905>.
23. Guinier A. X-Ray Diffraction: In Crystals, Imperfect Crystals, and Amorphous Bodies. Mineola, NY, USA: Dover Publications, 2013.
24. Huang WJ, Sun R, Tao J, Menard LD, Nuzzo RG, Zuo JM. Coordination-dependent surface atomic contraction in nanocrystals revealed by coherent diffraction. Nature Materials 2008; 7(4): 308-313. < 10.1038/nmat2132 >.
25. Xiong S, Lee S-Y, Noyan IC. Average and local strain fields in nanocrystals. Journal of Applied Crystallography 2019; 52: 262-273. < 10.1107/S1600576719000372 >.
26. Least-Square Atomic Strain, Li Group. <http://li.mit.edu/Archive/Graphics/A/annotate_atomic_strain/Doc/main.pdf>
27. Stukowski A, Markmann J, Wissmüller J, Albe K. Atomistic origin of microstrain broadening in diffraction data of nanocrystalline solids. Acta Materialia 2009; 57(5): 1648:1654. < 10.1016/j.actamat.2008.12.011>.