Olive Road Science
Materials data analysis

X-ray diffraction analysis of a ZnO nanopowder

Sample report · phase identification, profile fitting, crystallite size, microstrain and lattice parameters

This is a demonstration. The diffraction pattern was generated by computer from known values and then analysed exactly as a client's measurement would be. It shows the format and depth of a real report, and because the true values are known it also shows how closely the analysis recovers them.

1. Summary of results

Quantity	Result	Value used to make the data
Phase	ZnO, hexagonal wurtzite (9 reflections indexed)	ZnO, wurtzite
Lattice parameter a	3.24979 ± 0.00003 Å	3.2498 Å
Lattice parameter c	5.20653 ± 0.00007 Å	5.2066 Å
Crystallite size (Williamson–Hall)	28.9 ± 0.3 nm	28.0 nm
Microstrain (Williamson–Hall)	0.130 ± 0.004 %	0.120 %
Crystallite size (Scherrer, mean of peaks)	19.6 nm	see section 4
Weighted profile residual R_wp	3.9 %	–

2. Measured pattern and fitted profile

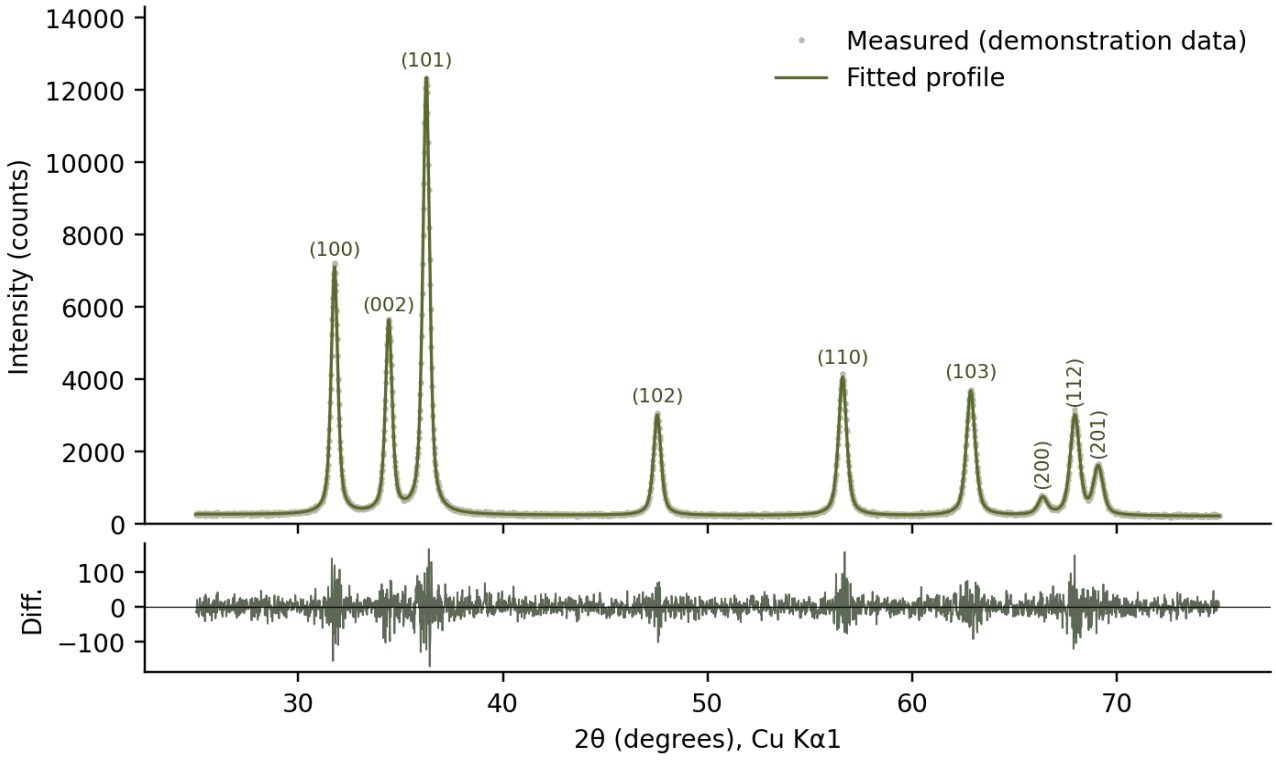


Figure 1. Measured pattern (grey points), fitted profile (green line) and their difference (lower panel). All nine reflections between 25° and 75° are indexed to wurtzite ZnO; no unassigned peaks remain.

3. Peak table

hkl	2θ (°)	d (Å)	FWHM (°)	Corrected breadth (°)	Scherrer size (nm)
(100)	31.769 ± 0.001	2.8144	0.381 ± 0.002	0.373	22.1
(002)	34.423 ± 0.001	2.6033	0.389 ± 0.002	0.381	21.8
(101)	36.254 ± 0.000	2.4758	0.394 ± 0.001	0.386	21.6
(102)	47.541 ± 0.001	1.9111	0.437 ± 0.004	0.430	20.2
(110)	56.597 ± 0.001	1.6249	0.476 ± 0.003	0.469	19.2
(103)	62.859 ± 0.001	1.4772	0.511 ± 0.003	0.505	18.4
(200)	66.377 ± 0.004	1.4072	0.540 ± 0.014	0.534	17.8
(112)	67.949 ± 0.001	1.3784	0.539 ± 0.004	0.533	18.0
(201)	69.089 ± 0.002	1.3584	0.558 ± 0.007	0.552	17.5

4. Crystallite size and microstrain

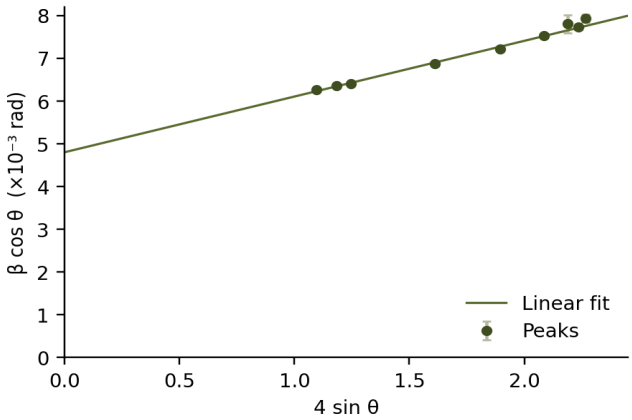


Figure 2. Williamson–Hall plot. The intercept gives the crystallite size and the slope gives the microstrain.

The Scherrer equation attributes all of the broadening to size, so it gives a smaller value (19.6 nm on average) that decreases at higher angles. The Williamson–Hall analysis separates the two contributions and gives 28.9 nm with 0.13 % microstrain. For this sample the Williamson–Hall value is the one to report.

5. Methods

The pattern (25–75° 2θ, step 0.02°, Cu Kα1, λ = 1.5406 Å) was fitted in one step with nine pseudo-Voigt peaks on a quadratic background, weighting each point by its counting statistics. Peak widths were corrected for an instrumental broadening of 0.08° by subtraction in quadrature. Crystallite size was calculated from the Scherrer equation with K = 0.9 and from a weighted Williamson–Hall fit, $\beta \cos\theta = K\lambda/D + 4\varepsilon \sin\theta$. Lattice parameters were refined by least squares against all nine peak positions. Uncertainties are one standard deviation from the fits.

6. Notes for a real measurement

In a client project the instrumental broadening is taken from a standard measured on the same diffractometer, Kα2 is handled in the profile model, and the analysis is extended to Rietveld refinement where the data quality supports it. The delivered package also contains the processed data and the figures in vector format.