

PDFgui tutorial

Eleven worked examples from a Ni cell
to a faulted CdSe nanoparticle

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29 September 2026 · Business Lounge, CC Academia



Engine: <https://www.diffpy.org/products/pdfgui.html>



How the room should have been organized

Install + copy

~10 min

PDFgui binary and the enumerated example folders.

Session 1 — guided

120 min

Work examples 0–5 together before coffee.

Session 2 — DIY

90 min

Examples 6–10 with help. Complex cells, r-series, nanoparticles.

Each folder

README + .ddp

Data, instructions, and a pre-made project as the answer key.

How the room is actually organized

Install + copy

~0 min

PDFgui binary and the enumerated example folders.

Session 1 — guided

45-60 min

Work examples 0–1 together.

Session 2 — DIY

at own time

Examples 2–10 with help. Complex cells, r-series, nanoparticles.

Each folder

README + .ddp

Data, instructions, and a pre-made project as the answer key.

Eleven examples in full tutorial

#0

Simulate Ni & BaTiO₃

#1

Ni X-ray refinement

#2

Ni neutron refinement

#3

Ni X+n co-refinement

#4

Ni / Si mixture

#5

Ni T-series

#6

LaMnO₃ complex cell

#7

LaMnO₃ T-series

#8

Cu(Ir_{1-x}Cr_x)₂S₄ r-box-car

#9

CeO₂ bulk vs nano

#10

CdSe NP wurtzite

Two examples in mini tutorial

#0

Simulate Ni & BaTiO₃

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Ni X-ray refinement

#2

Ni neutron refinement

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Ni X+n co-refinement

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Ni / Si mixture

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CeO₂ bulk vs nano

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CdSe NP wurtzite

Simulate Ni — then break the knobs

Goal: learn the calculator before you trust a residual.

Fm-3m · a = 3.524 Å · Ni at 0,0,0 · Uiso = 0.005 · project 00-nickel.ddp

1. Build the 300 K Ni cell; expand if you want a supercell.
2. Calculate X-ray and neutron G(r) from 0.01–10 Å. Overlay (offset = 0).
3. Copy the neutron calc: scale 0.2; Qmax = 15 Å⁻¹; r to 100 Å.
4. On the 100 Å curve: Qdamp = 0.05, then spdiameter = 20 Å. Notice they look alike.
5. Set stepcut = 5.25 Å. Use Calculate bond lengths / angles on the phase.

BaTiO₃, partials, and chemical contrast

Goal: probe choice and occupancy models are not cosmetics.

Load from CIF. Projects 00-BaTiO₃.ddp and 00-nickel-02.ddp

1. Simulate BaTiO₃ X-ray vs neutron at $U_{iso} = 0.0005$ then $0.005 \text{ \AA}^2$.
2. Ask which probe sees oxygen. Change Included pairs to Ti–O (partial PDF).
3. Ni neutron: replace one site by Au (25 %).
4. Duplicate all Ni, set 4/8 to Au, occ Ni 0.75 / Au 0.25 on every site.
5. Compare random solid solution vs a distinct Au site. Contrast is the experiment.

Refine Ni X-ray, 300 K

Goal: a first real residual, with and without correlated motion.

X7B / NSLS, Perkin Elmer · $Q_{\max} = 22 \text{ \AA}^{-1}$ · $Q_{\text{damp}} = 0.045$

1. Set up and refine without delta parameters.
2. Read R_w , the difference curve, and the correlation table.
3. Turn on correlated-motion parameters and refine again.
4. The first peak should tighten. If everything else moves, you over-parameterised.

Refine Ni neutron, 300 K

Goal: same cell, different contrast and a kinder Qdamp.

NPDF / LANSCE TOF · $Q_{\max} = 27 \text{ \AA}^{-1}$ · $Q_{\text{damp}} = 0.012$

1. Repeat #1 on the neutron $G(r)$.
2. Compare lattice, Uiso and delta with the X-ray fit.
3. Neutron Q_{damp} is smaller — field of view is longer. Do not mix the two numbers.

Co-refine X-ray and neutron Ni

Goal: one structure, two datasets, two instrument envelopes.

X-ray Qdamp 0.045 · neutron Qdamp 0.012 · shared cell

1. One phase, two datasets. Share lattice, positions, U. Do not share Qdamp or dscale.
2. Execute and inspect which parameters the two probes actually agree on.
3. Think of failure modes: bad relative scale, residual container, different Qmax ripples.

Two-phase Ni + Si mixture

Goal: phase fractions without inventing a new crystal.

Ni Fm-3m $a \approx 3.52 \text{ \AA}$ · Si F-43m $a \approx 5.43 \text{ \AA}$ · APS 6-ID MAR345

1. Fit pure Ni. Fit pure Si. Park those parameters.
2. On the mixture: two phases, one dataset. One dscale; two pscale (or the reverse — pick a convention and keep it).
3. Report the phase content. Ask when this is better than a Rietveld weight fraction.

Ni temperature series

Goal: the T-macro and linked fits.

X7B · 80–500 K in 20 K steps · $Q_{\max}$ 22 · Q_{damp} 0.045

1. Seed from the 300 K fit.
2. Fits → Macros → T-series. Files must be in temperature order; each output seeds the next.
3. Plot $a(T)$, $U_{\text{iso}}(T)$. PDFgui will not invent a phase transition you did not parameterise.
4. Limitation: one starting symmetry for the whole movie.

LaMnO₃ — a cell with opinions

Goal: Pnma, four sites, then anisotropic U.

Pnma · a,b,c ≈ 5.74, 7.71, 5.54 Å · NPDF 300 K · Q_{max} 32 · Q_{damp} 0.012

1. Build La, Mn, O1, O2 from the fractional coordinates given in the README.
2. Refine with Uiso on all sites. Read the residual at the first Mn–O shell.
3. Promote selected sites to anisotropic Uij under Pnma constraints.
4. More parameters must earn their keep on chemistry, not only on R_w.

LaMnO₃ 300–1100 K

Goal: two structural transitions, visible in the refined parameters.

Same Pnma setting. Files: 300, 550, 650, 700, 720–750, 800, 880, 980, 1050, 1100, 1150 K.

1. T-macro, files strictly in T order.
2. Plot lattice and U vs T. Ask which traces break at the known transitions.
3. A cubic average at high T does not erase a local JT distortion — look at low-r if the high-r cell looks ‘simple’.

Box-car r-fits on Cu(Ir,Cr)₂S₄

Goal: estimate a short-range correlation length from $R_w(r)$.

Fd-3m · $a \approx 9.80 \text{ \AA}$ · 100 K · APS 11-ID-C · start from 08-cics-fd3m-rdep.ddp

1. Fit 20–40 $\text{\AA}$ cubic, refine Qdamp and Qbroad, delta fixed at 0.
2. Park those values. Fit 1.5–40 $\text{\AA}$ with only delta1 free — high-r works, low-r fails below $\sim 10 \text{ \AA}$.
3. Macros $\rightarrow$ r-series: max 5–25 step 1; min 1–21 step 1 (4 $\text{\AA}$ windows, 1 $\text{\AA}$ shift).
4. Run the linked box-cars. Plot R_w vs index. That decay is your correlation-length estimate.

CeO₂ bulk versus nano

Goal: spdiameter is a shape envelope, not a miracle.

Fm-3m · $a \approx 5.41 \text{ \AA}$ · X17B3 / NSLS · $Q_{\text{max}} 24.5$ · $Q_{\text{damp}} 0.045$

1. Refine bulk CeO₂. Park Q_{damp} .
2. Apply the same model to nano-CeO₂. Watch high- r die while the model keeps oscillating.
3. Release spdiameter. Diameter should be physical. Ask what the residual still wants (strain, non-sphericity, reconstructed surface).
4. Compare .chi raw patterns. Size is already a Scherrer story; PDF adds the real-space envelope.

CdSe nanoparticle, wurtzite

Goal: Qdamp and size fight; stacking faults hide in a single-range fit.

P63mc · $a \approx 4.30 \text{ \AA}$, $c \approx 7.01 \text{ \AA}$ · APS 6-ID · Qmax 19 · Qdamp start 0.045

1. Bulk wurtzite model, Qdamp fixed. Try several r-ranges — parameters will walk.
2. On one range: Qdamp fixed vs free. If the answer jumps, those parameters are correlated with size / stacking.
3. Proper Qdamp comes from a bulk standard in the same geometry, not from the nanoparticle itself.
4. A single cell will not invent 50 % stacking faults. That is a later model (see Masadeh et al., PRB 76, 115413).

House rules at the machine

- 01 Save a .ddp after every idea that worked.
- 02 Never refine Qdamp and spdiameter together on the sample of interest.
- 03 If $|\text{correlation}| > 0.8$, one of those knobs is lying.
- 04 A pretty difference curve at 2–10 Å with a wild lattice is not a structure.
- 05 When stuck, calculate the PDF of the model with all sliders at default — look first.