

# Combining X-ray, neutron and electron diffraction with spectroscopies and first principle energy computation for material science research

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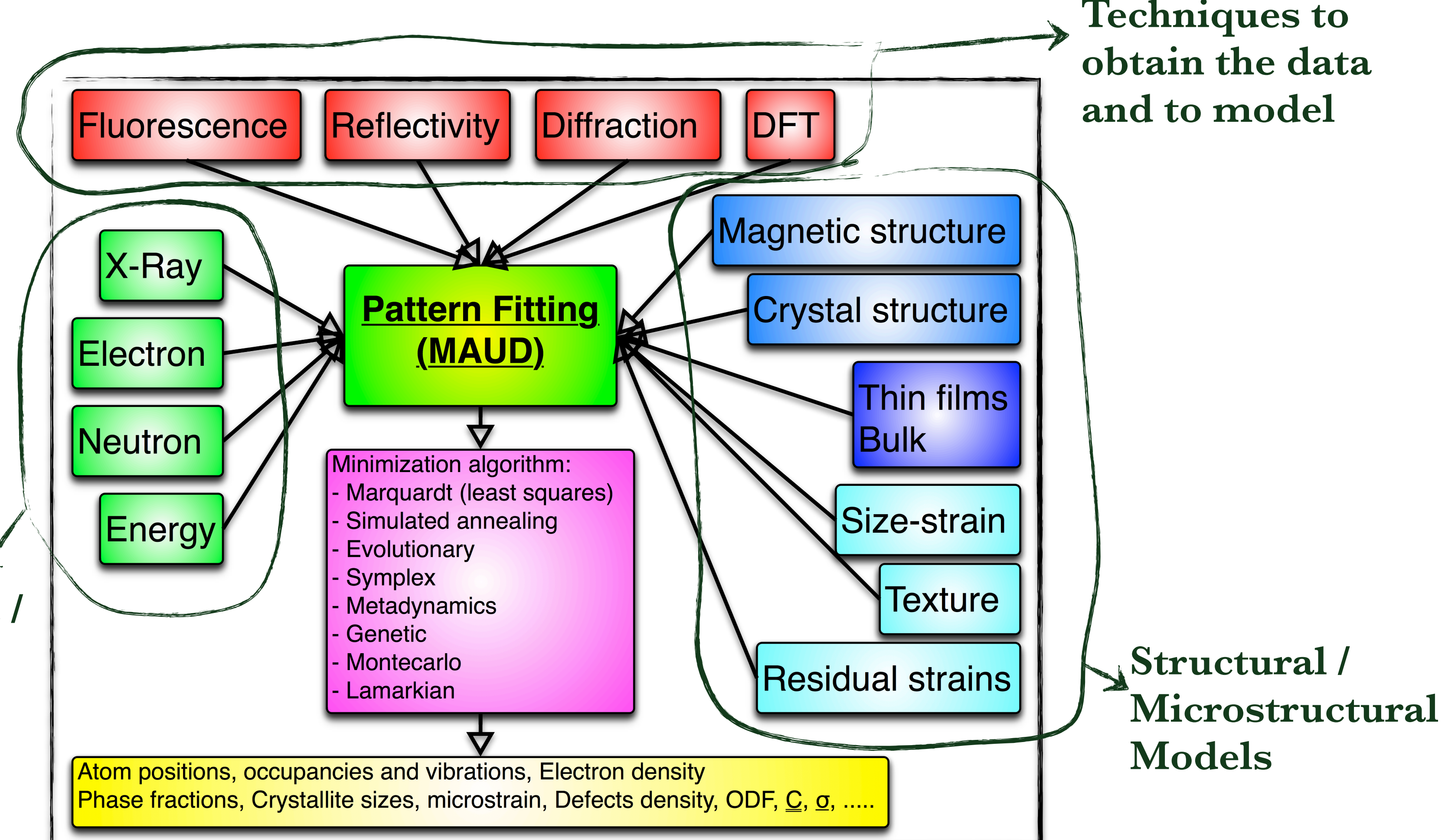
MAUD: <http://www.ing.unitn.it/~maud>

**The project:**

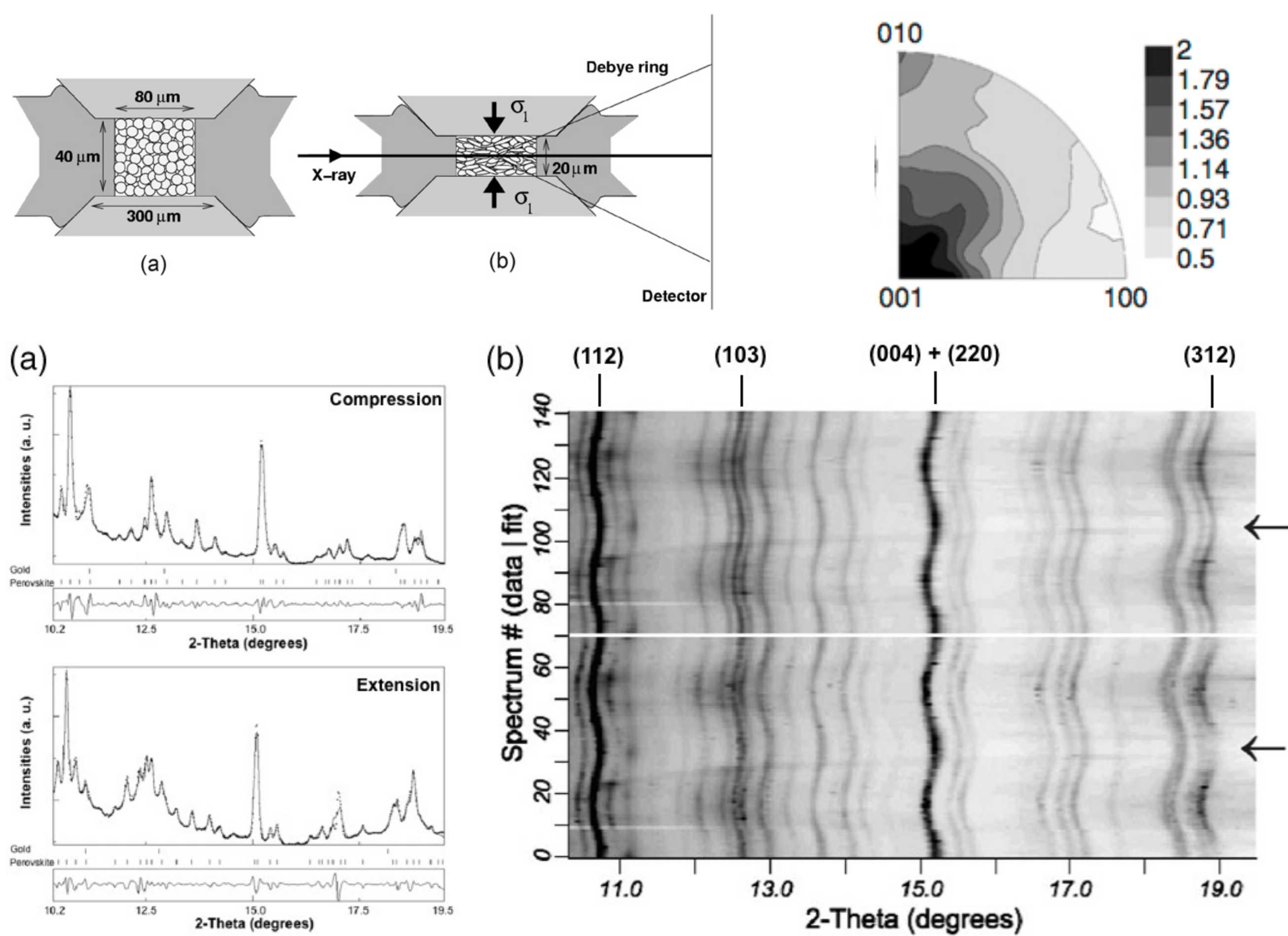
- Combined analysis: state of the art (already assessed)
  - Microstructure: phase analysis, size-strain, texture, residual stresses
  - Thin films, grazing angle and reflectivity
  - Crystal structure, fragments, algorithms
  - X-ray, neutron, electron (kinematic)
- Combined analysis: actual work (under testing)
  - Energy minimization / DFT (Density Functional Theory)
  - Debye/PDF (Pair Distribution Function)
  - X-ray fluorescence, EDXS
  - Magnetic structure/texture
  - Dynamical scattering (electron)
- Combined analysis: future work (to do)
  - Raman, EXAFS, NMR, IR....



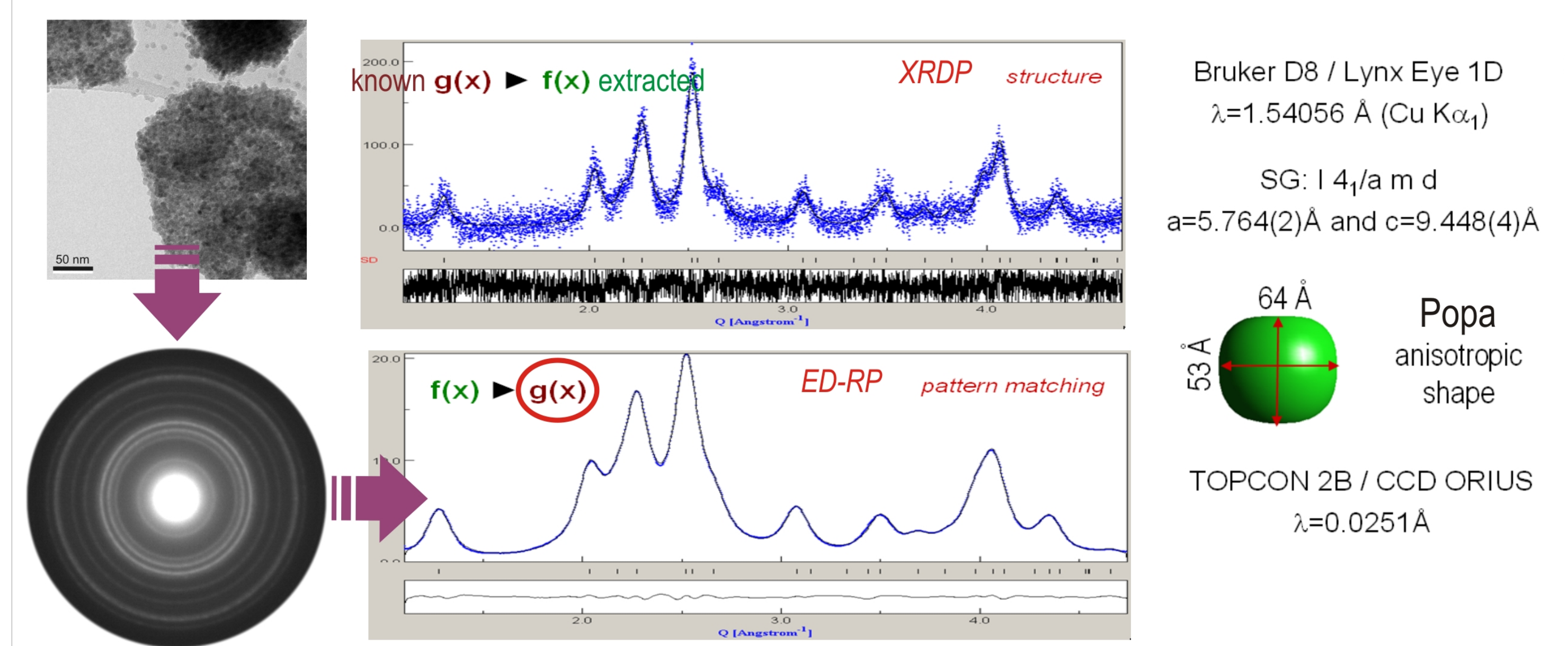
Data to fit / minimize



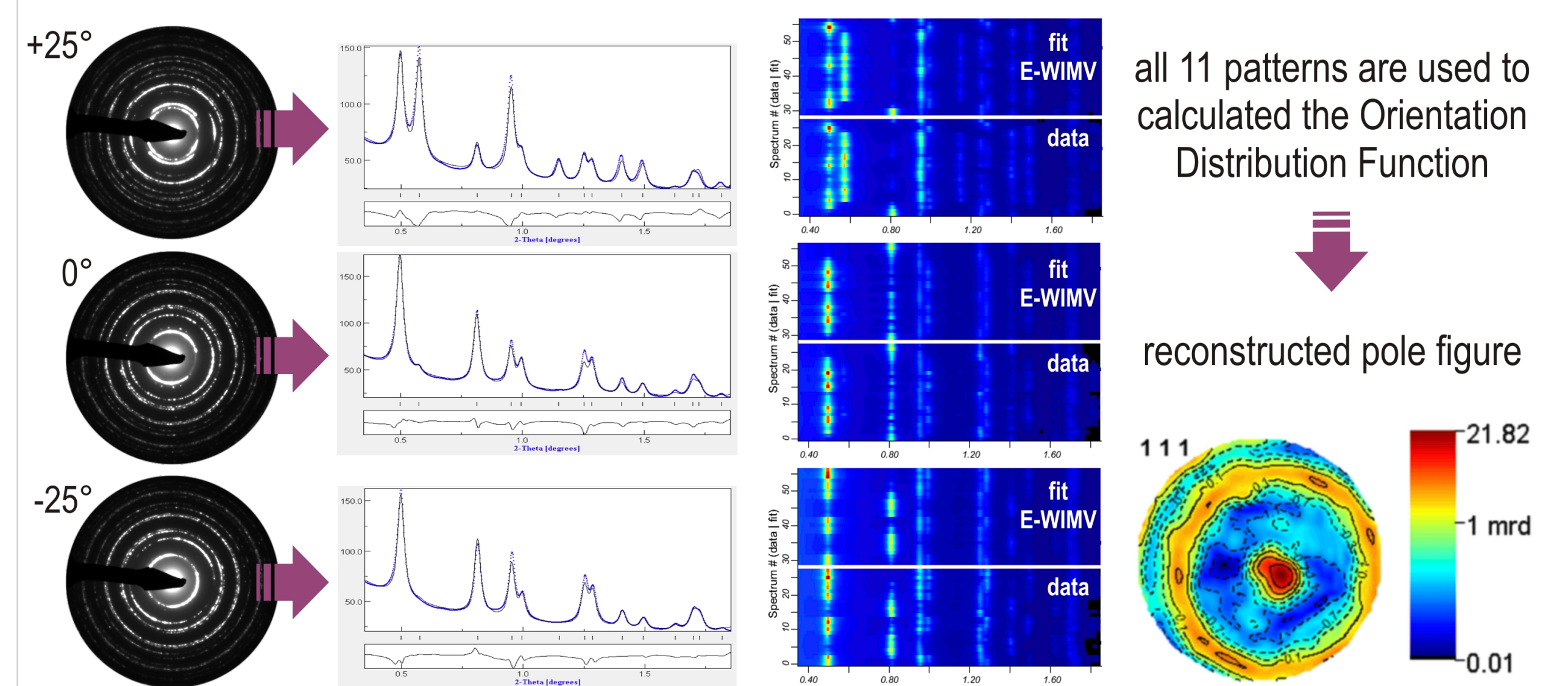
## MgSiO<sub>3</sub> at 43 GPa (Texture and Stresses)



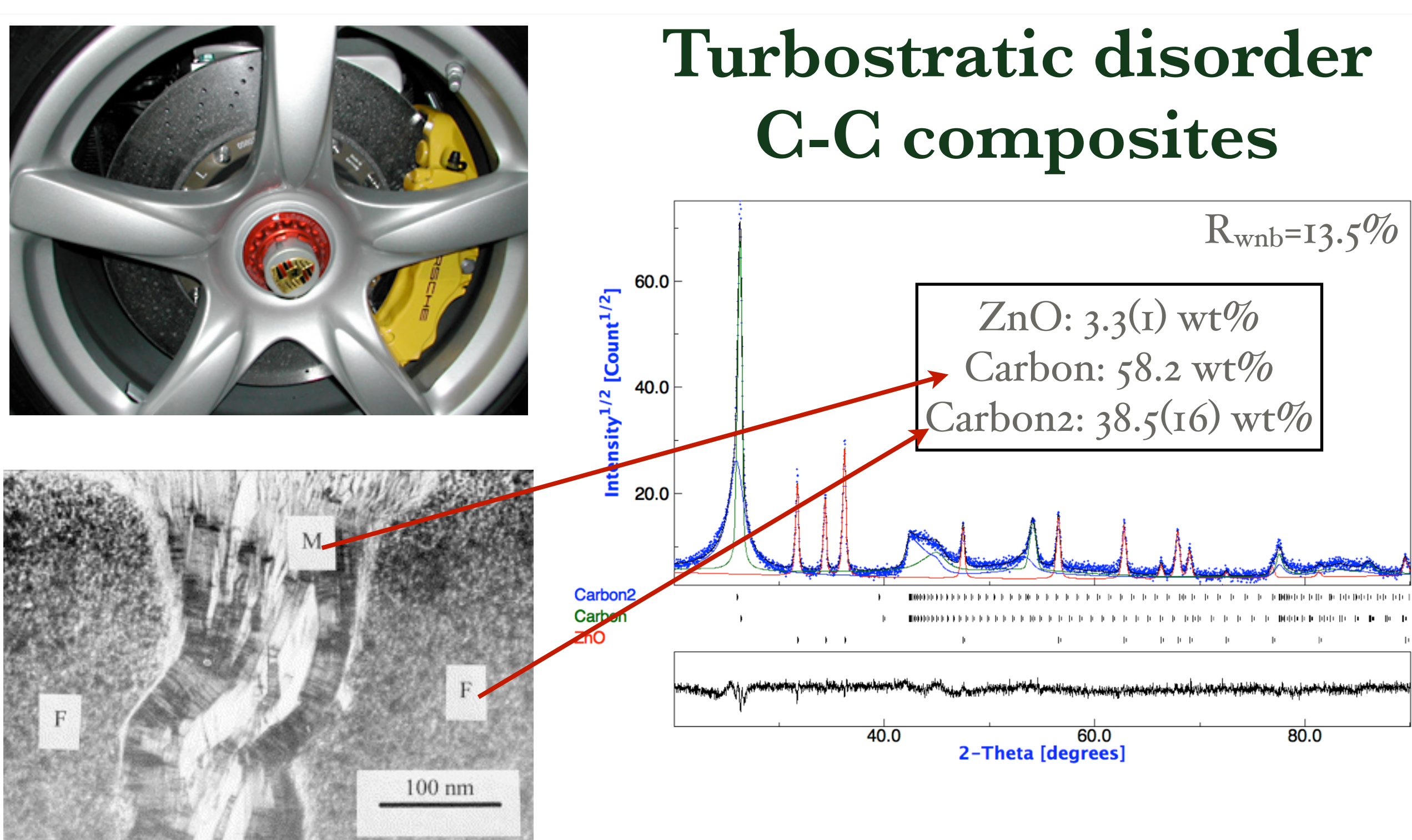
## Nano Mn<sub>3</sub>O<sub>4</sub>: Size-strain analysis (XRD + TEM)



## MgO thin film: Quantitative Texture Analysis by electron diffraction

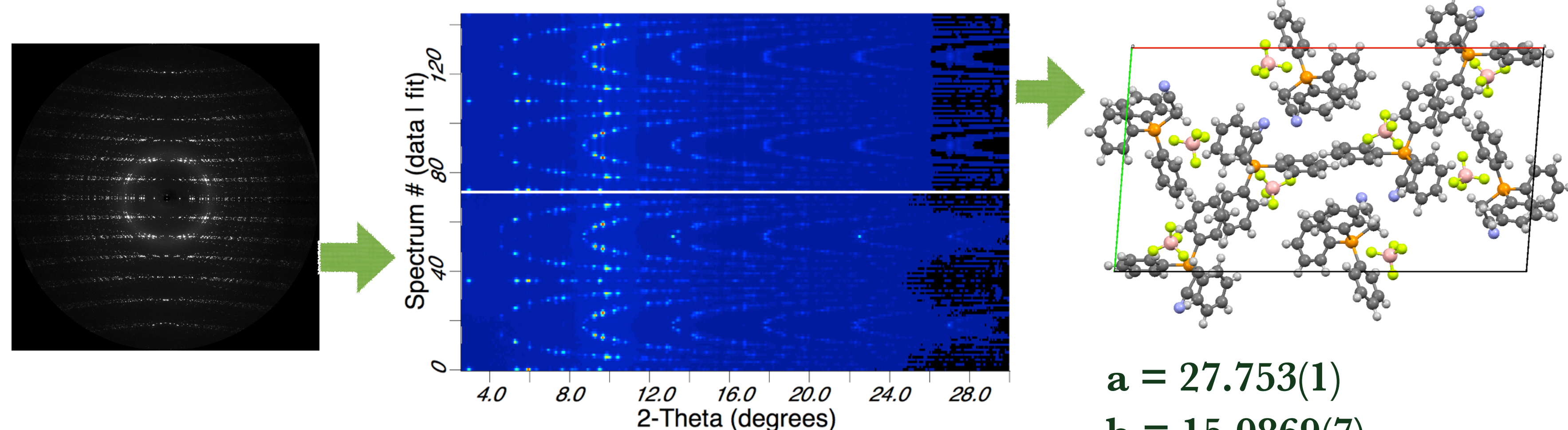


## Turbostratic disorder C-C composites



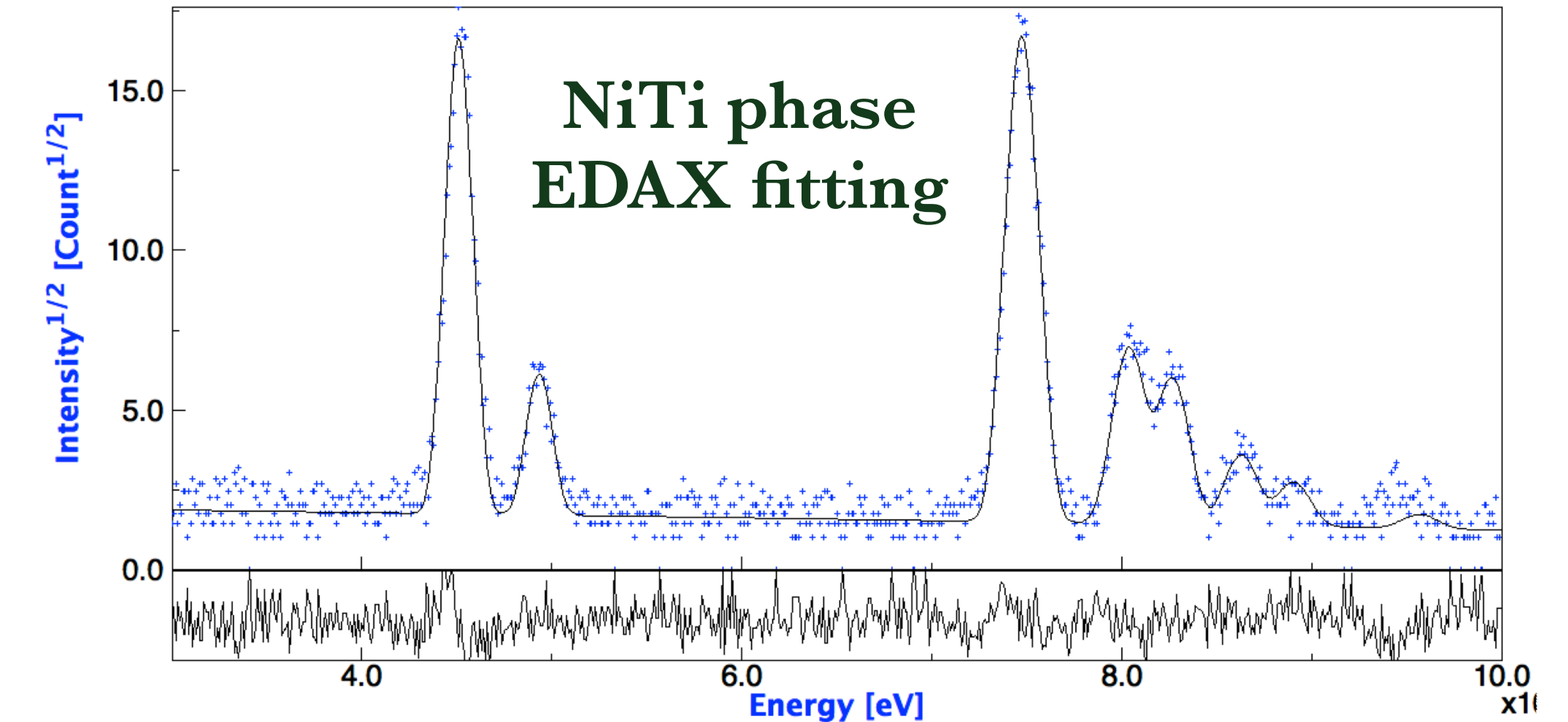
## [P(Ph)<sub>3</sub>CH<sub>2</sub>CN]BF<sub>4</sub> structure solution using texture

Fibers in capillary spinned, one image shot



Monoclinic P2<sub>1</sub>/c (Solution: Lamarkian algorithm & Standard Functions + energy DFT by Abinit)

## NiTi phase EDAX fitting



## Combining diffraction & reflectivity (ESQUI)

