

# What's new in R's `plotnine` function analysis

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# Whole Powder Pattern Fitting

- "Rietveld" becoming a catch-all term
  - Including structure-less fitting methods (Pawley, LeBail)
  - Software generally supports several methods
  - Mature methods
- Pair Distribution Function analysis
  - Total Scattering
  - Long used for amorphous materials
  - Recently applied to nano / disordered structures
- Common concept – use all the available data
  - "Rietveld" analyses long range structure
  - Total Scattering looks also at short range structure

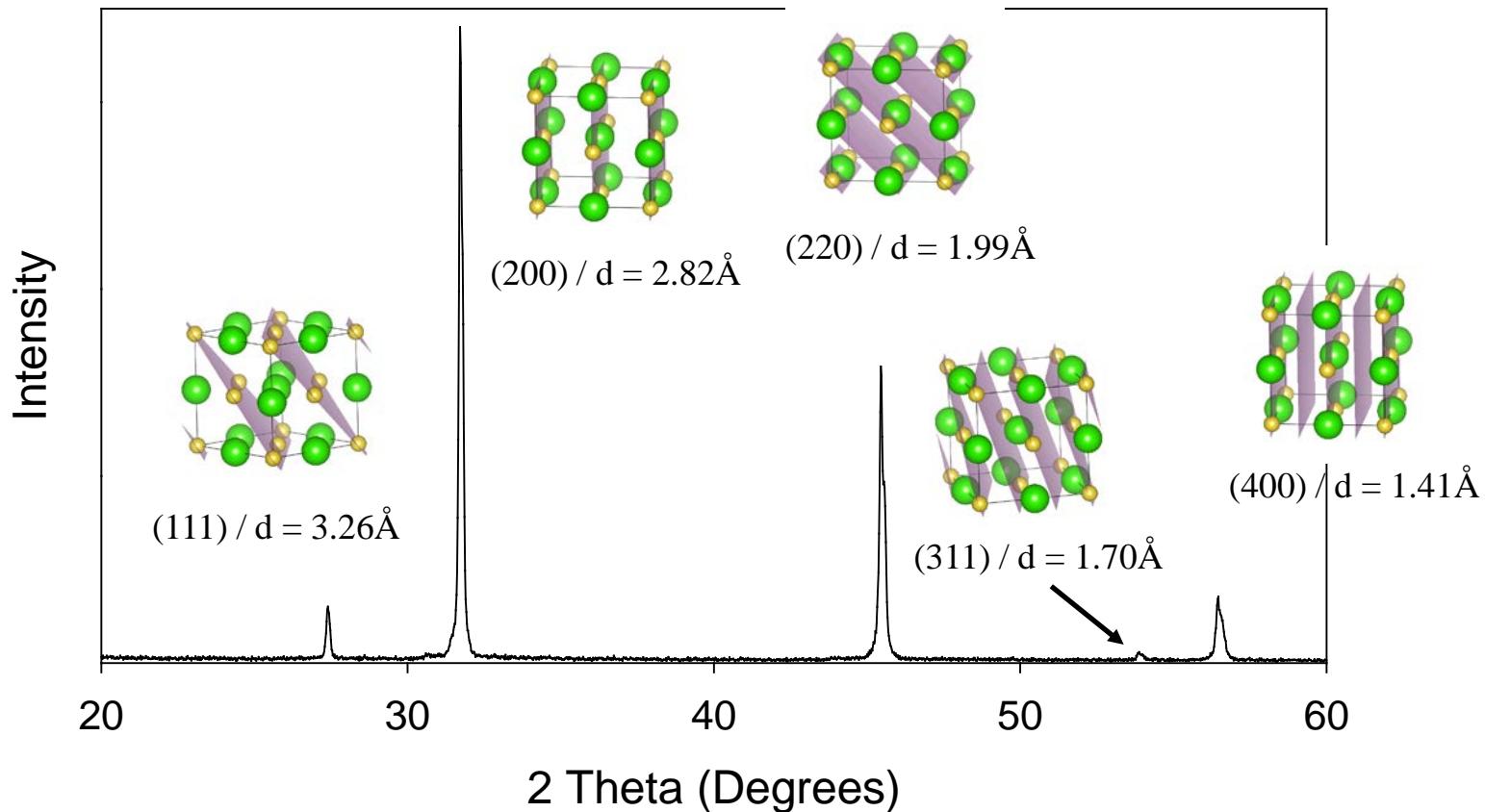
# Reminder

Peak positions

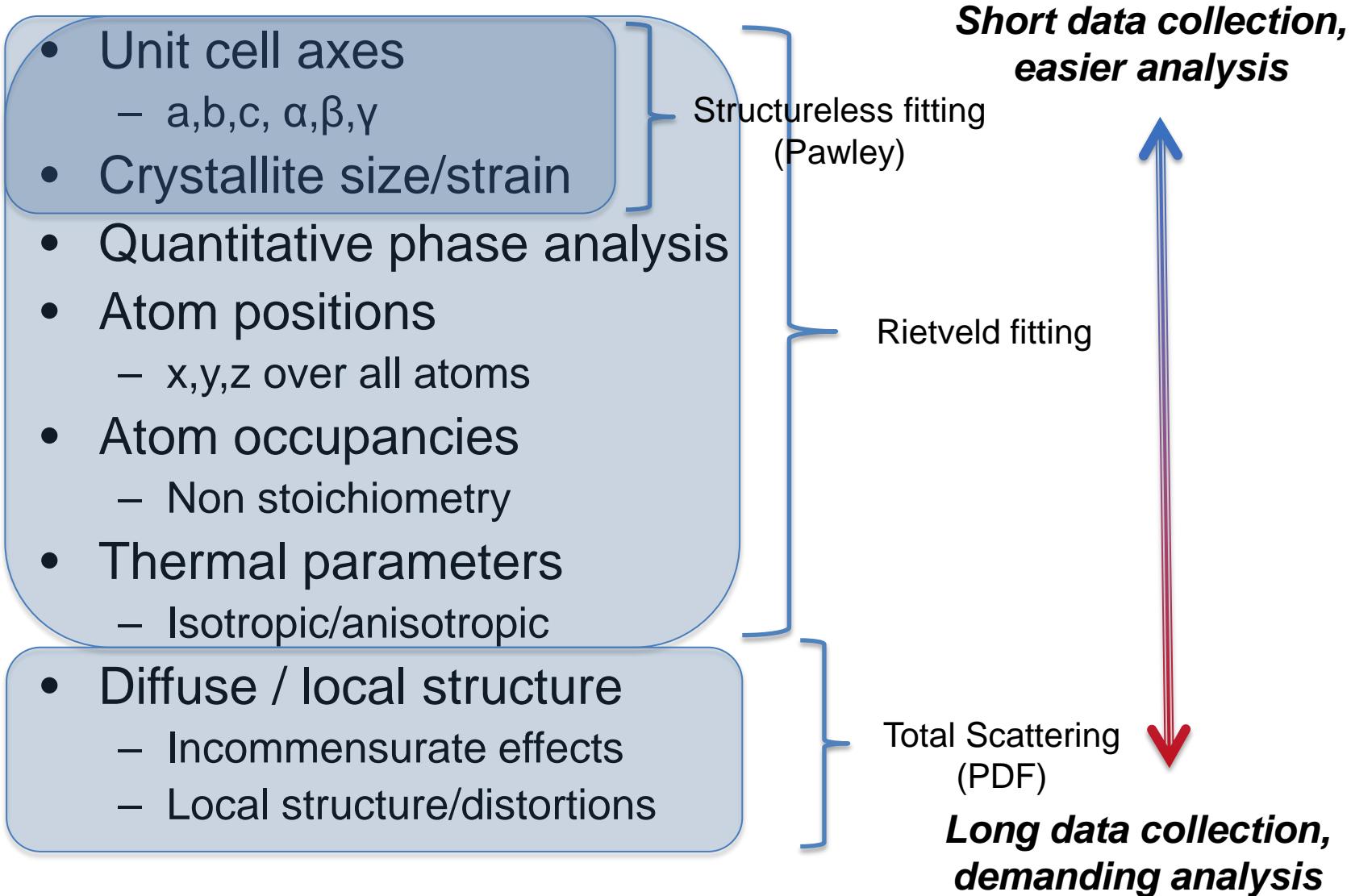
$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

Peak intensities

$$F_{hkl} = \sum_{n=0}^{n=N} f_n \exp 2\pi i (hu_n + kv_n + lw_n)$$



# Analysis Objectives



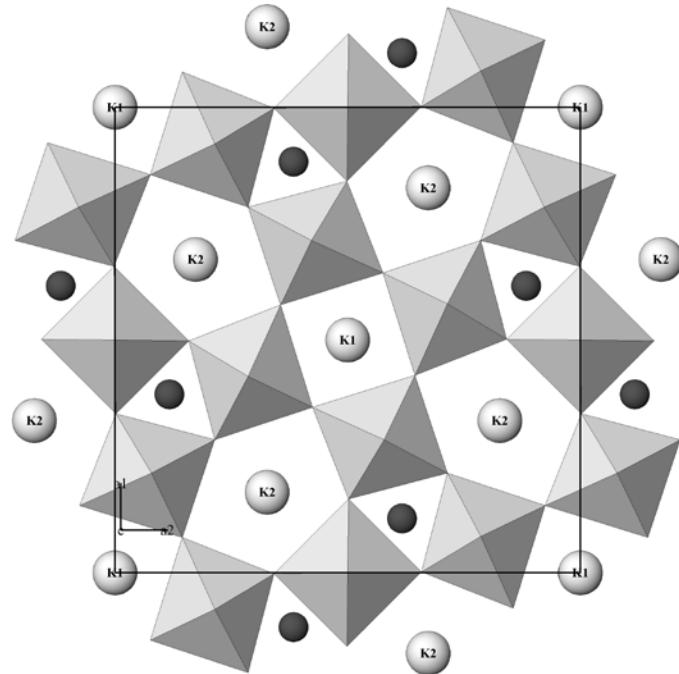
# **Example – K<sub>2</sub>Nb<sub>4</sub>O<sub>11</sub>**

# $\text{K}_2\text{Nb}_4\text{O}_{11}$

- Tetragonal Tungsten Bronze
- SG P4/mbm,  $a=12.58\text{\AA}$ ,  $c=3.98\text{\AA}$

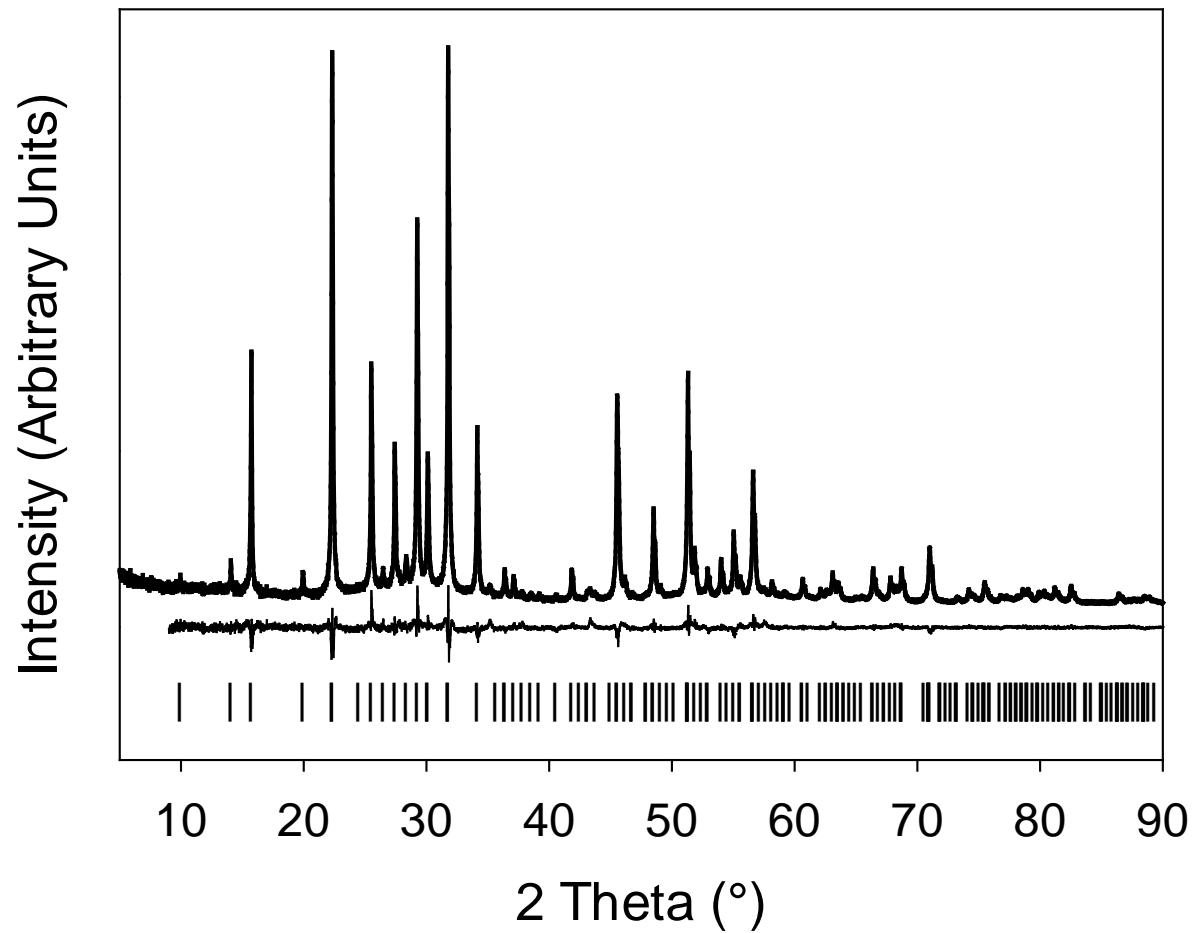
Site	Wychoff symmetry	X	Y	Z	Occupancy
Nb(1)	2b	0.00000	0.50000	0.50000	1.0000(41)
Nb(2)	8j	0.07555(9)	0.20818(9)	0.50000	1.0000(14)
Nb(3)	8i	0.1146(59)	0.3826(59)	0.00000	0.1136(17)
K(1)	2a	0.00000	0.00000	0.00000	0.8478(73)
K(2)	4g	0.32642(26)	0.17358(26)	0.00000	0.9386(37)
O(1)	2d	0.00000	0.50000	0.00000	1.0000
O(2)	8i	0.07726(71)	0.21432(69)	0.00000	1.0000
O(3)	4h	0.21251(54)	0.28749(54)	0.50000	1.0000
O(4)	8j	0.00276(44)	0.34014(70)	0.50000	1.0000
O(5)	8j	0.14462(52)	0.07645(67)	0.50000	1.0000

$$F_{hkl} = \sum_{n=0}^{N} f_n \exp 2\pi i (hu_n + kv_n + lw_n)$$



# $K_2Nb_4O_{11}$

- 7hr scan
- $R_{wp}=3.68$



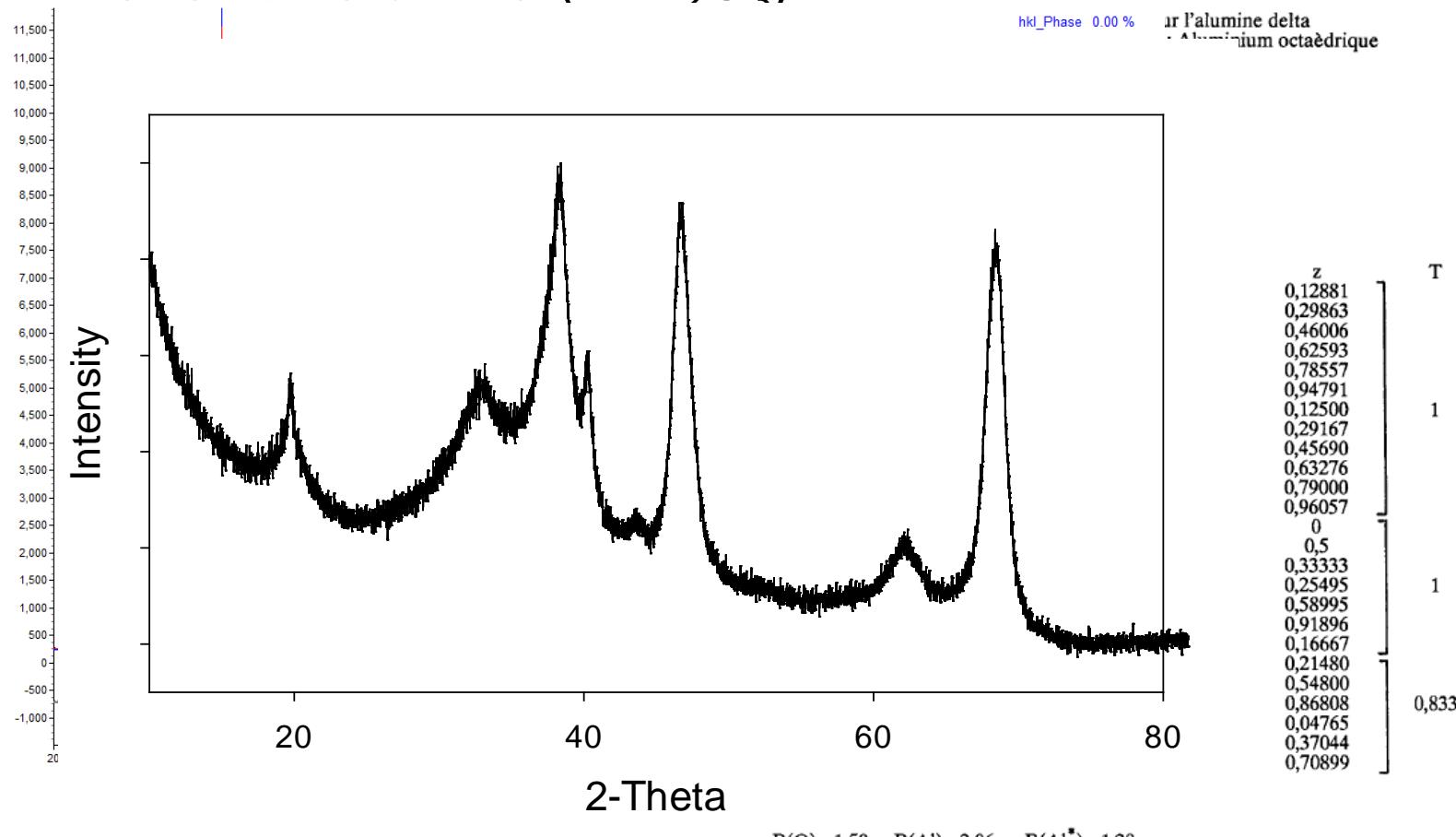
# Total Scattering – Al<sub>2</sub>O<sub>3</sub>

# Total Scattering (PDF)

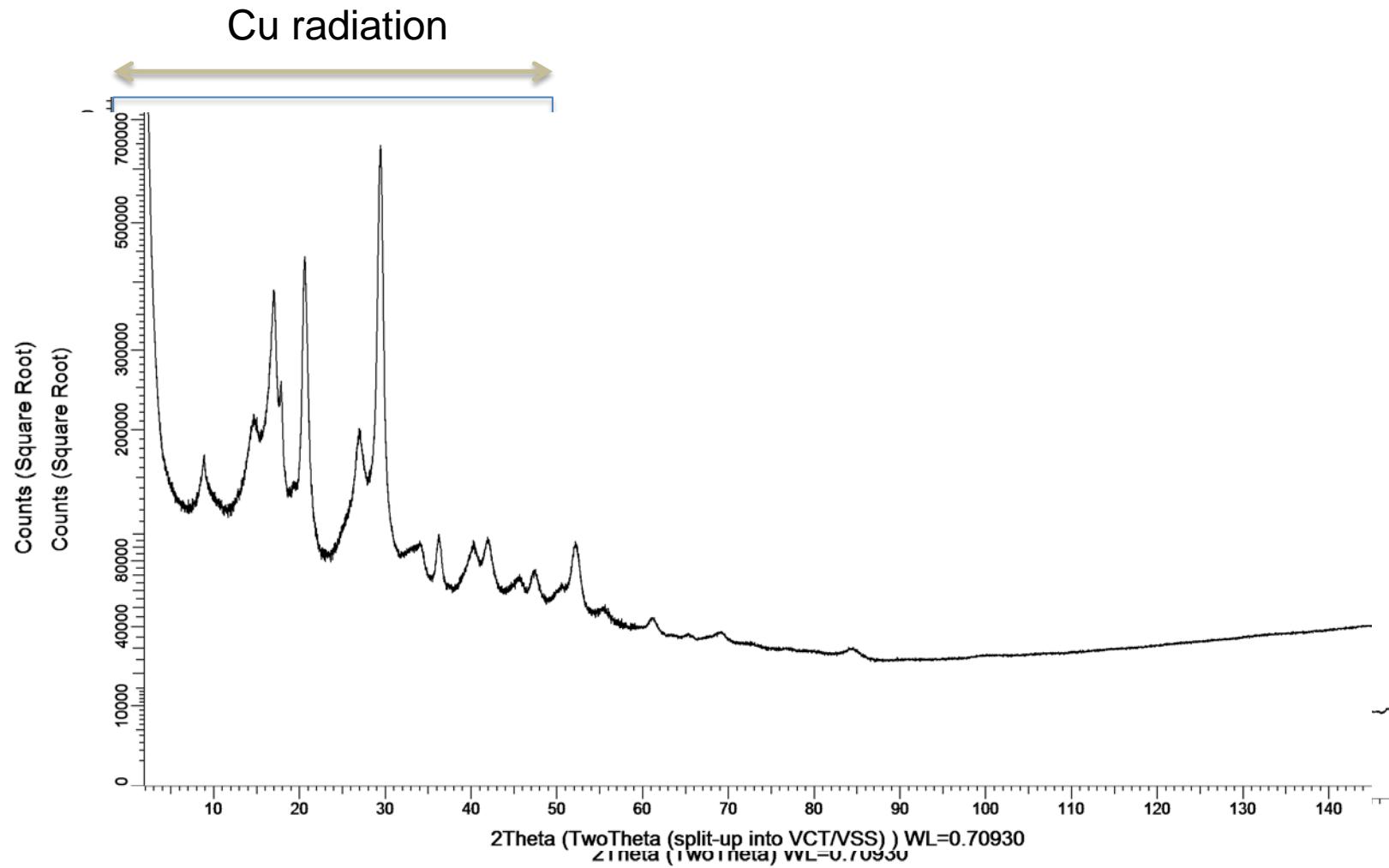
- Need much better data than for Rietveld
  - Good statistics over very large Q-range (d-spacing)
- Short wavelength ( $\lambda$ ) and long collection times
  - Synchrotron ideal
  - Possible in the lab (Mo/Ag radiation, 24hrs+ collection)
- Background subtraction required
  - Including sample holder
- Fourier transform whole dataset
  - Includes peaks and background

# Example – $\text{Al}_2\text{O}_3$

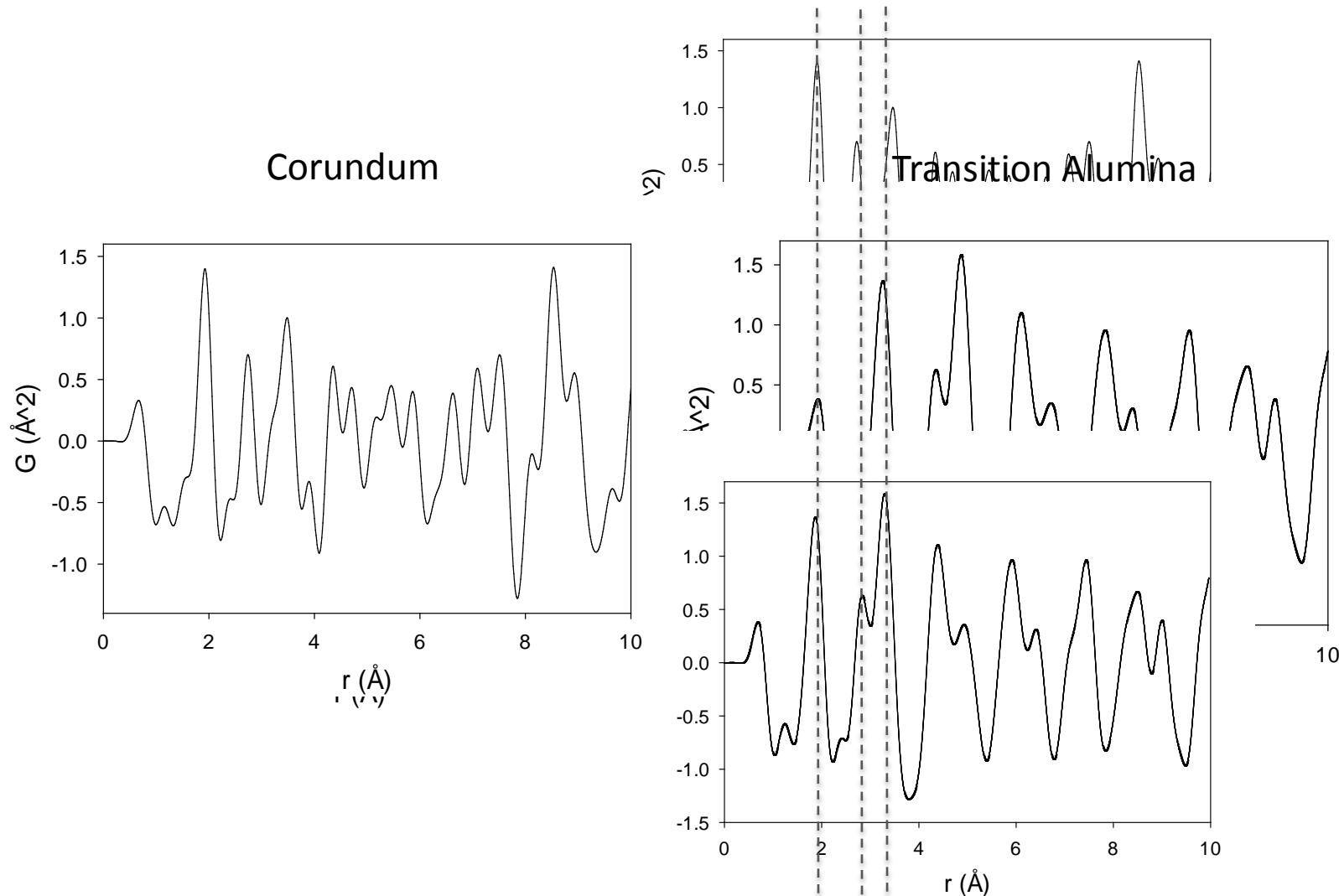
- Corundum
- Transition alumina ( $\delta\text{-Al}_2\text{O}_3$ )



# Total Scattering $\text{Al}_2\text{O}_3$



# Total Scattering $\text{Al}_2\text{O}_3$



# Instrumentation

# Instrumentation

- "Rietveld" analysis (Pawley / Rietveld)
  - Any diffractometer will do
  - 7 instruments at UiO (Cr, Cu, Mo)
  - 5 instruments at NTNU (Cu, Mo)
- Transmission mode better for organics
  - UiO better equipped
- Reflection mode better for oxides
  - UiO and NTNU both well equipped
- Total Scattering (PDF's)
  - UiO and NTNU both have new Mo-source instruments

**Thank you for your attention**