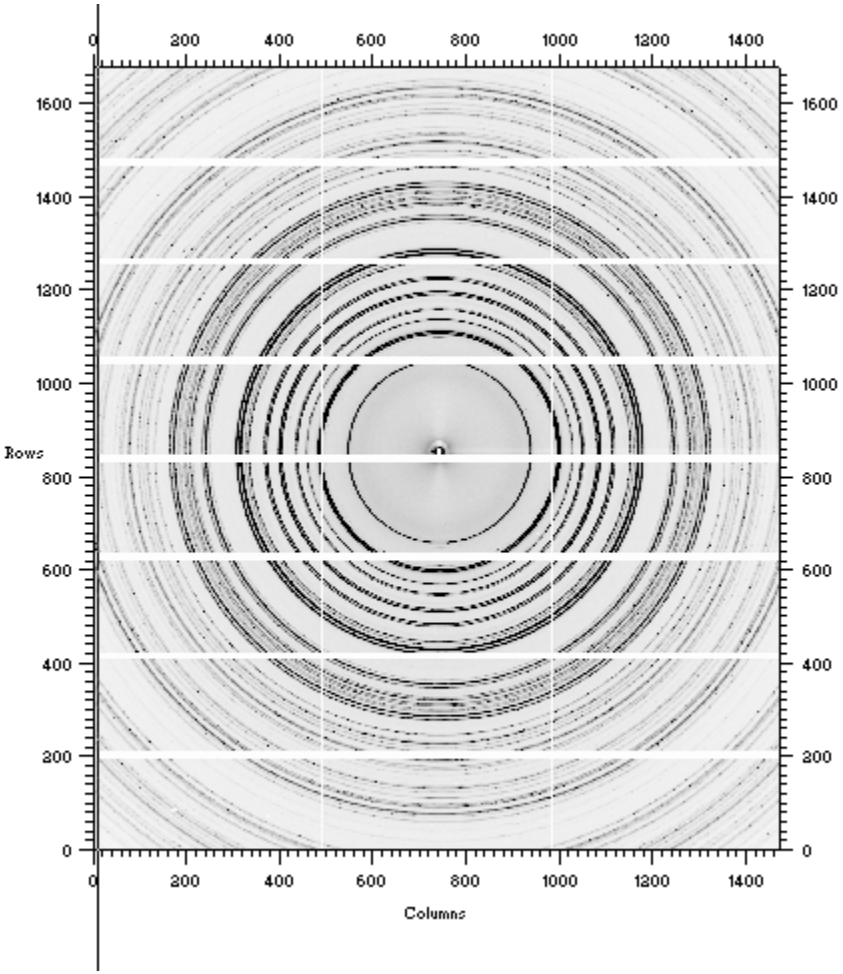
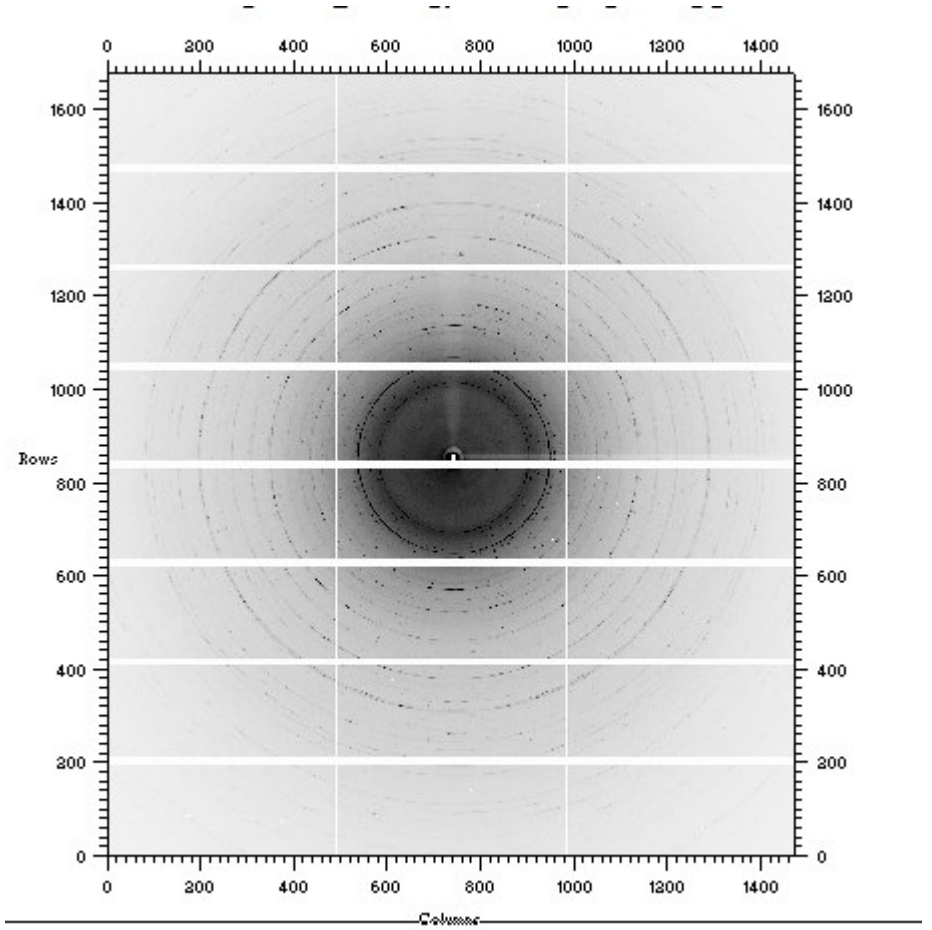
X-ray powder diffraction: Tutorial

- From raw data to integrated data
- Phase identification
- Pattern simulation
- Quantitative analysis
- Thermal expansion determination

2D raw data


0
200
400
600
800
1000
1200
1400
1600
Rows
Columns


0
200
400
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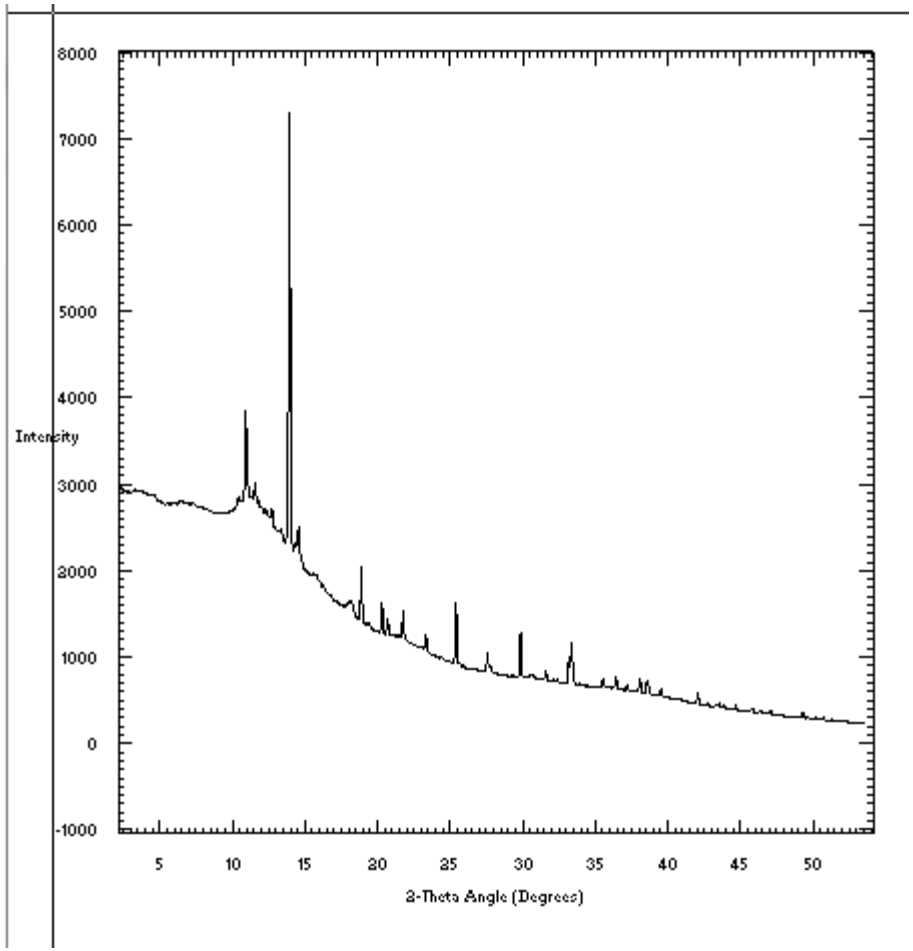
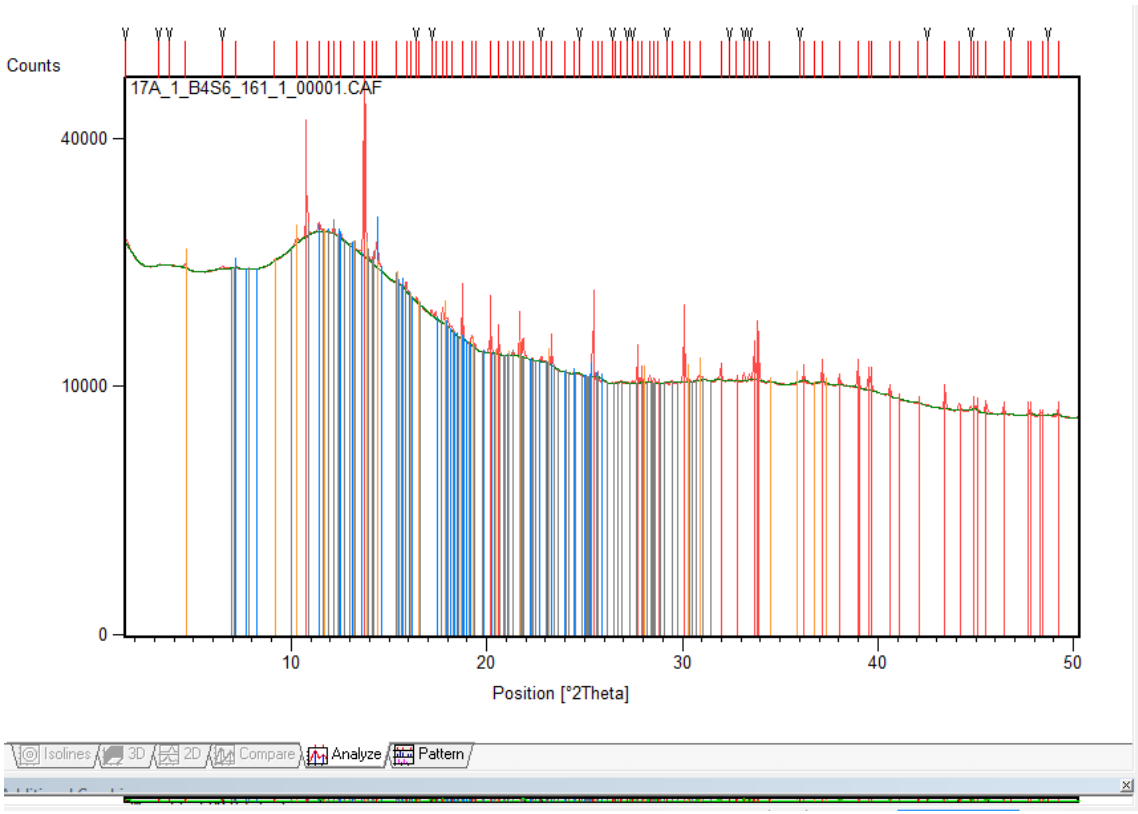
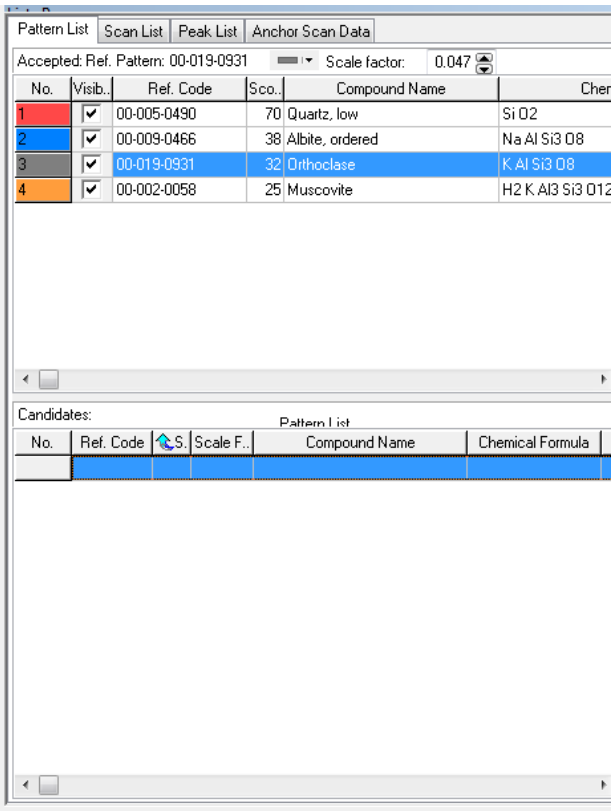
Rows
Columns

Integrated data

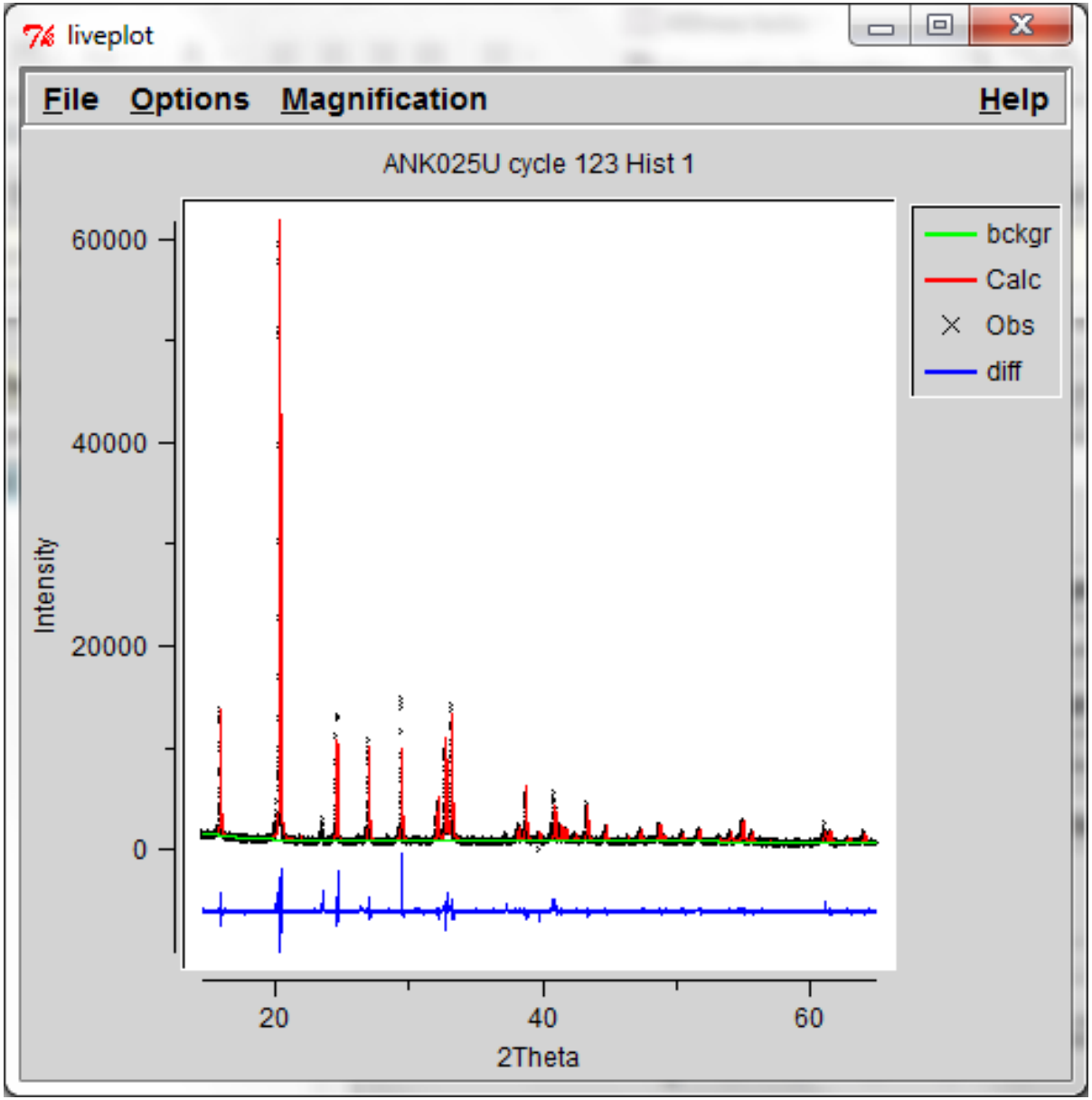


Phase identification

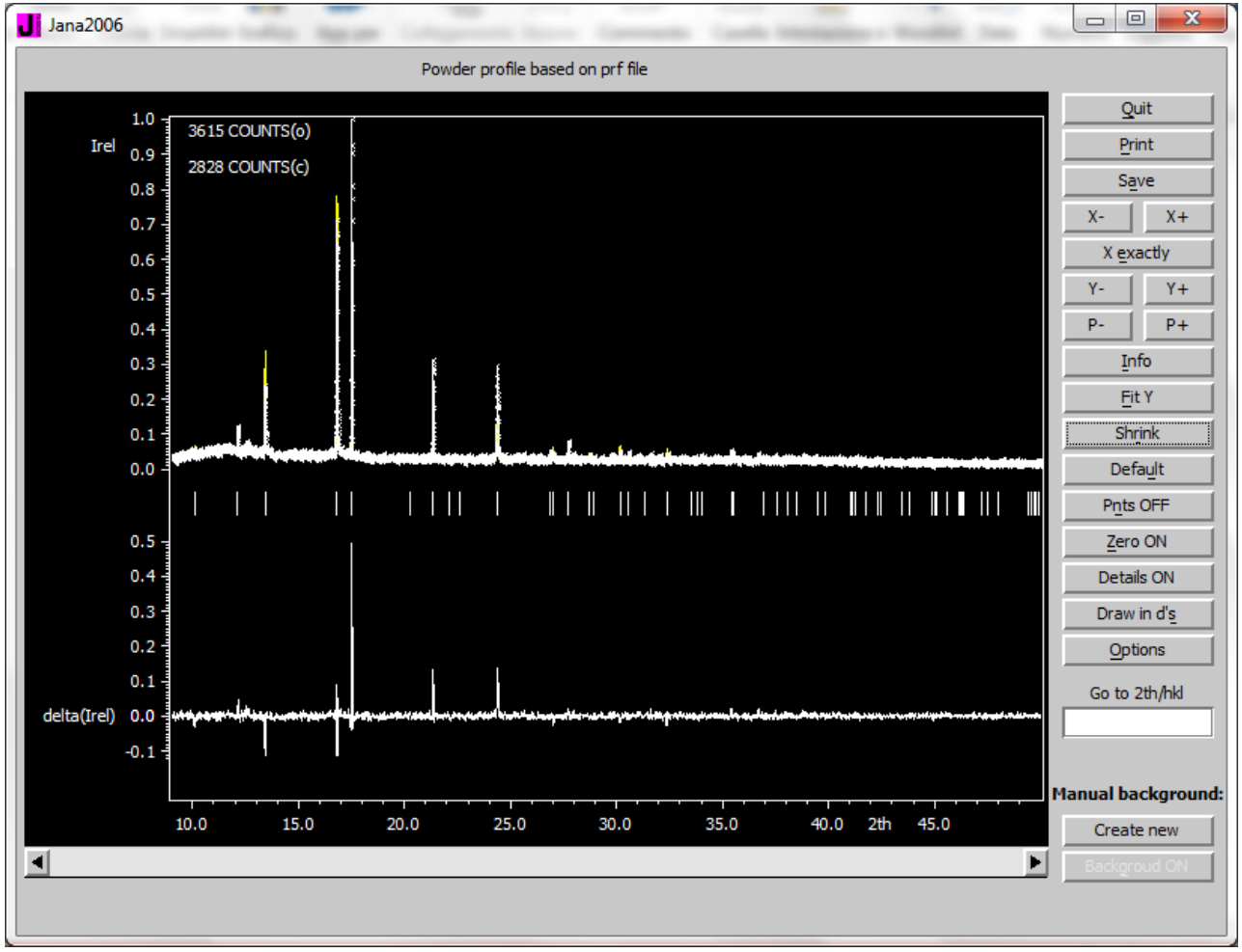


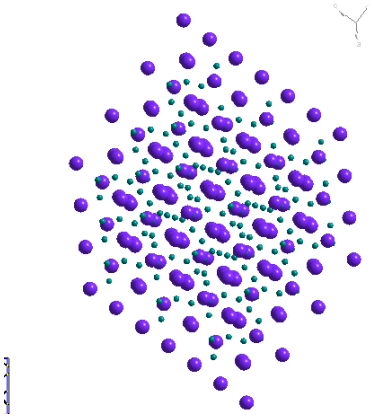


Pattern simulation – lattice parameter determination – quantitative analysis



Advanced: crystal structure determination





https://drive.google.com/open?id=0B0bfcGomFpKYekVET3J1cFVvdTA

- Software for data reduction (FIT2D)
- Software for Rietveld analysis (GSAS)

- Others: few programs for data conversion (i.e. ConvX…)
- Jana2006 (advanced, for structure determination, single crystal…)
- Diamond (old version, for structure visualization)
- Powdercell (for powder pattern simulation)