Automatic Identification of Regions of Neutron Diffraction Patterns Changing During Phase Transition

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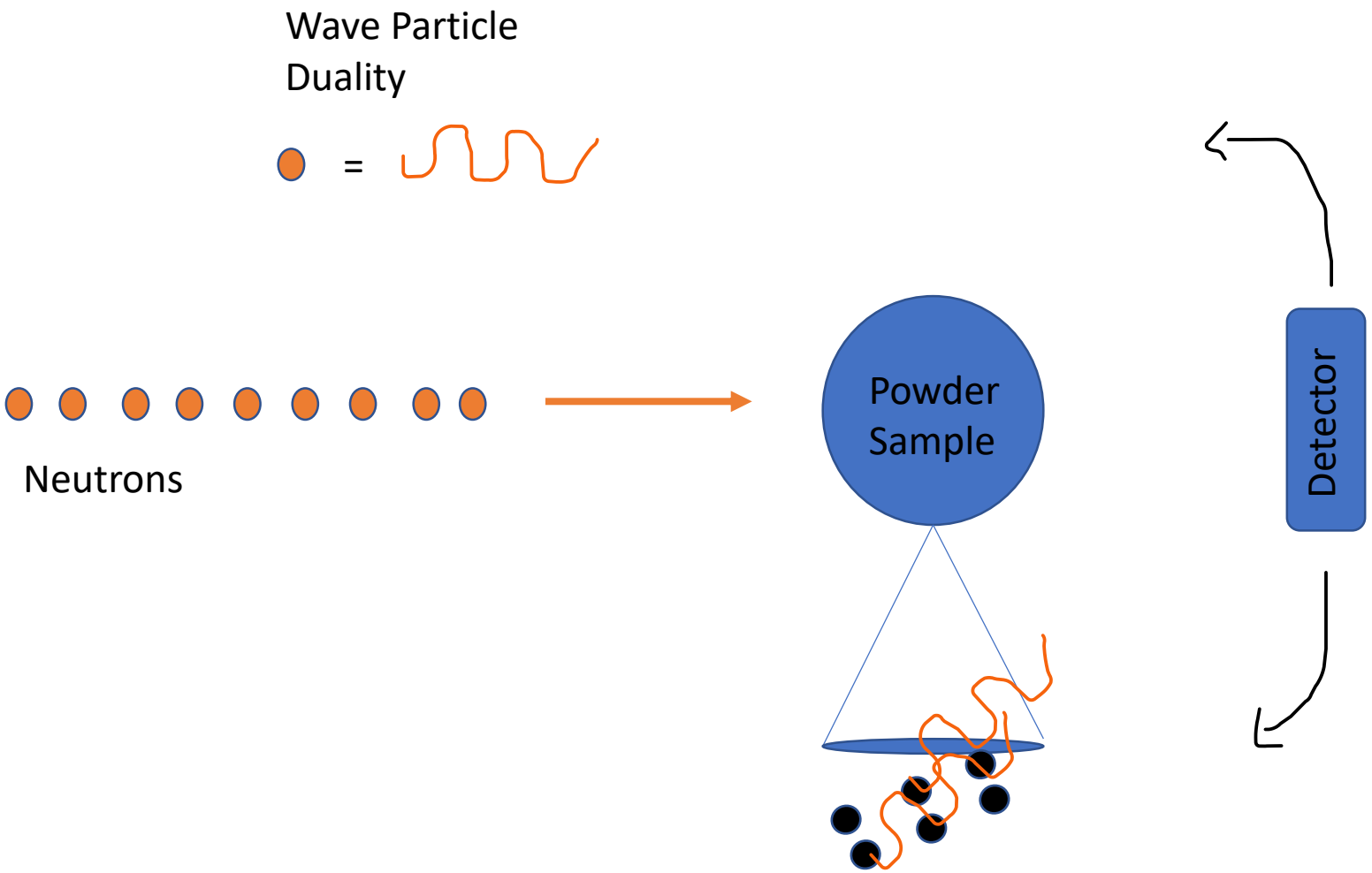
Neutron Scattering



Neutron Scattering

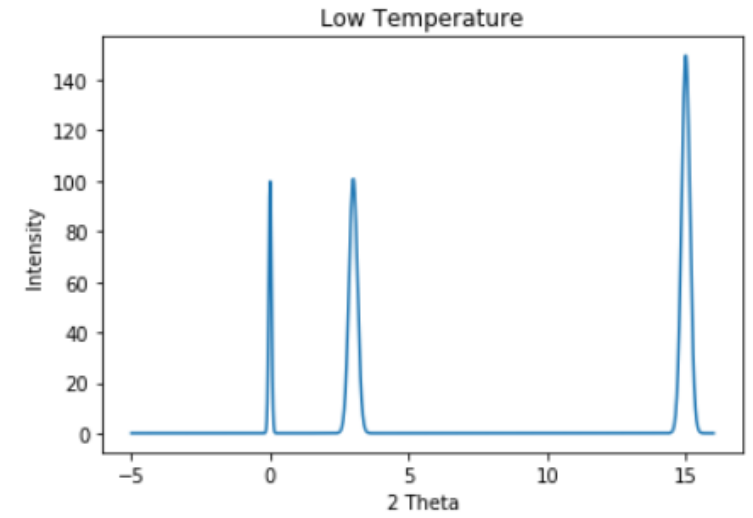
Change in powder temperature

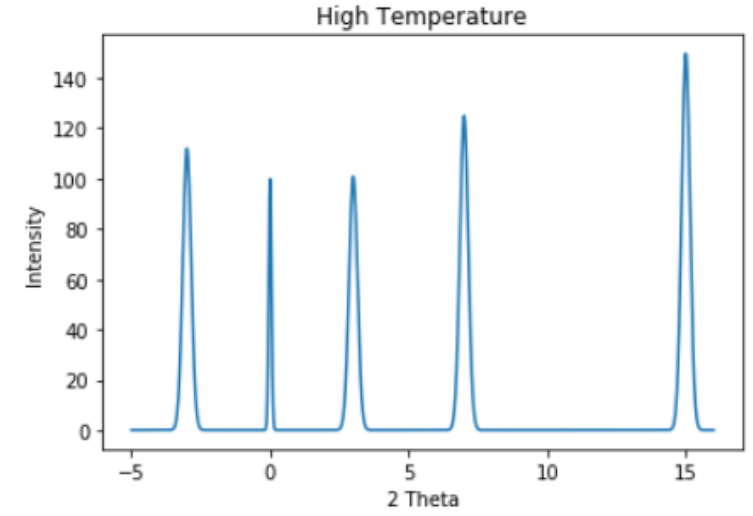
↓

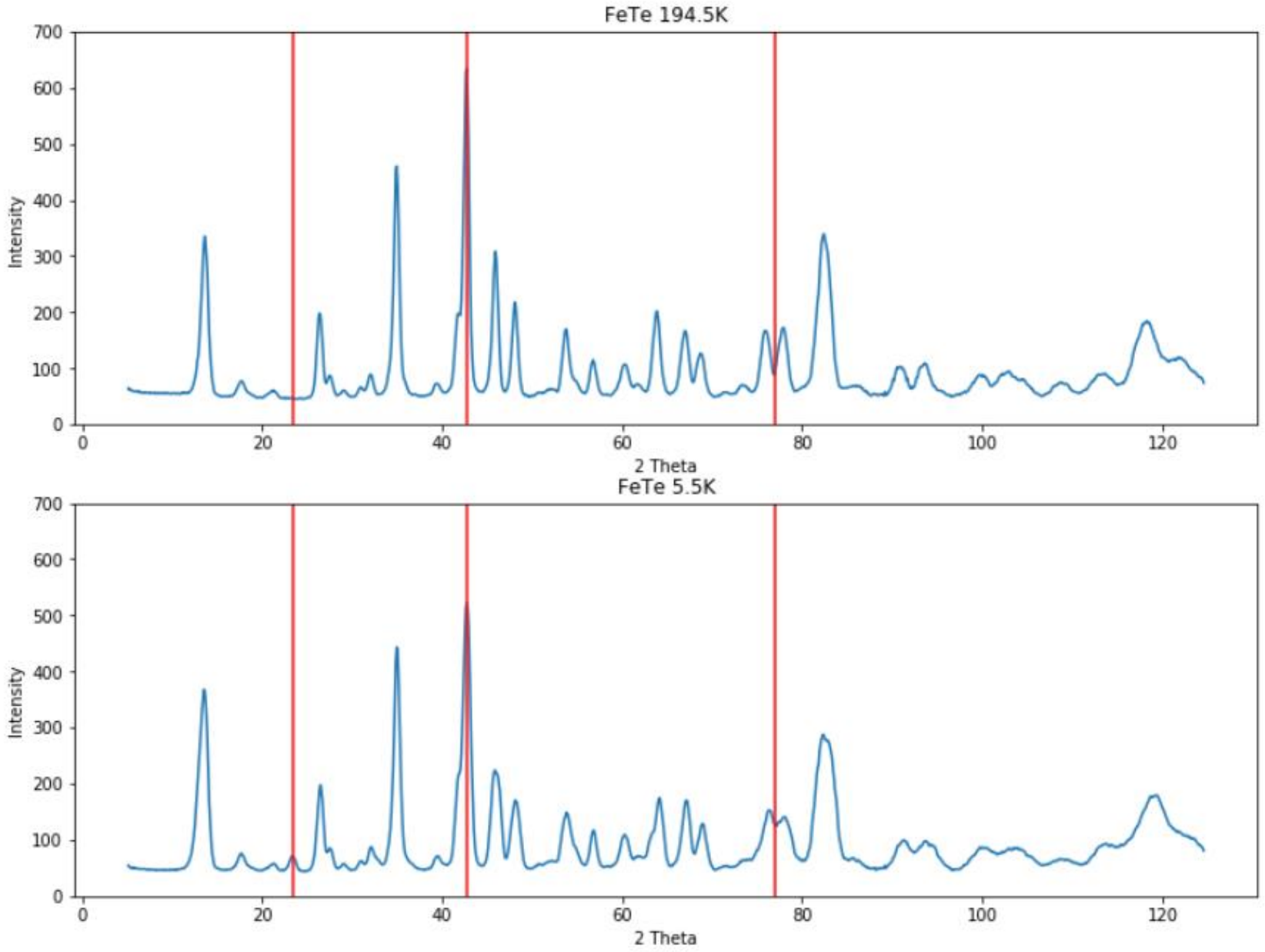
Change in powder structure

↓

Change in powder diffraction pattern



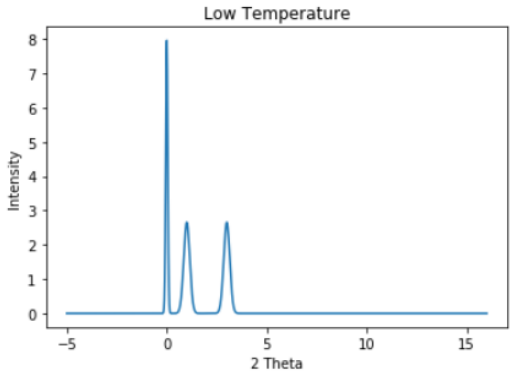


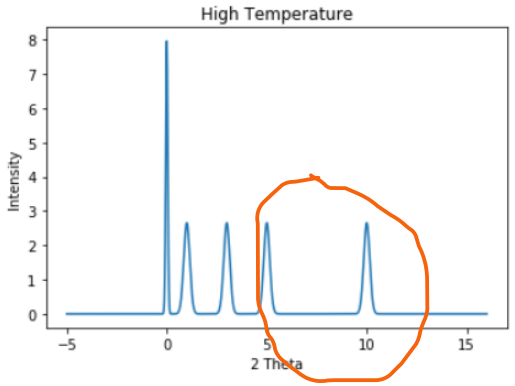


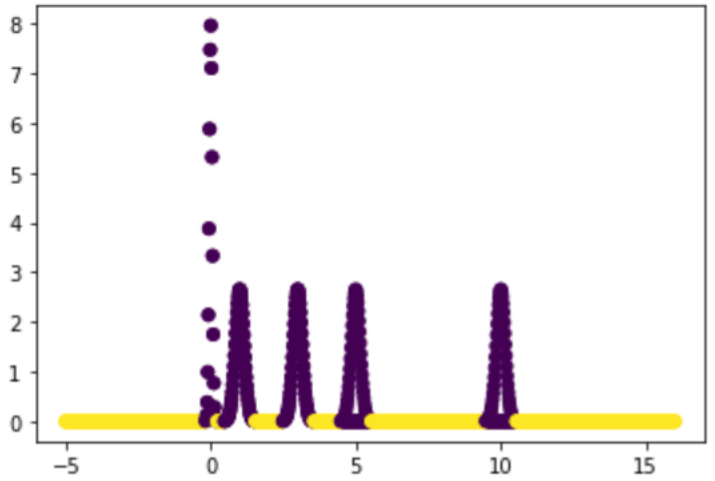
Real diffraction pattern data for FeTe (Iron Telluride) taken at Oak Ridge National Laboratory

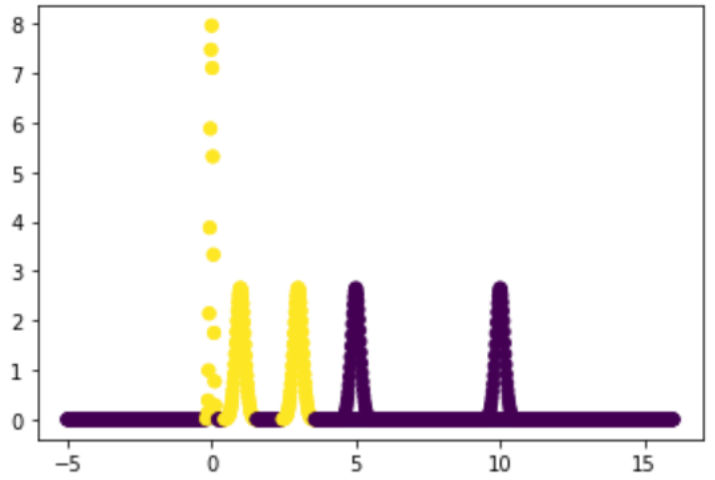
Gaussian Mixture Modelling

- Didn’t work
- Stuck in Local Minima







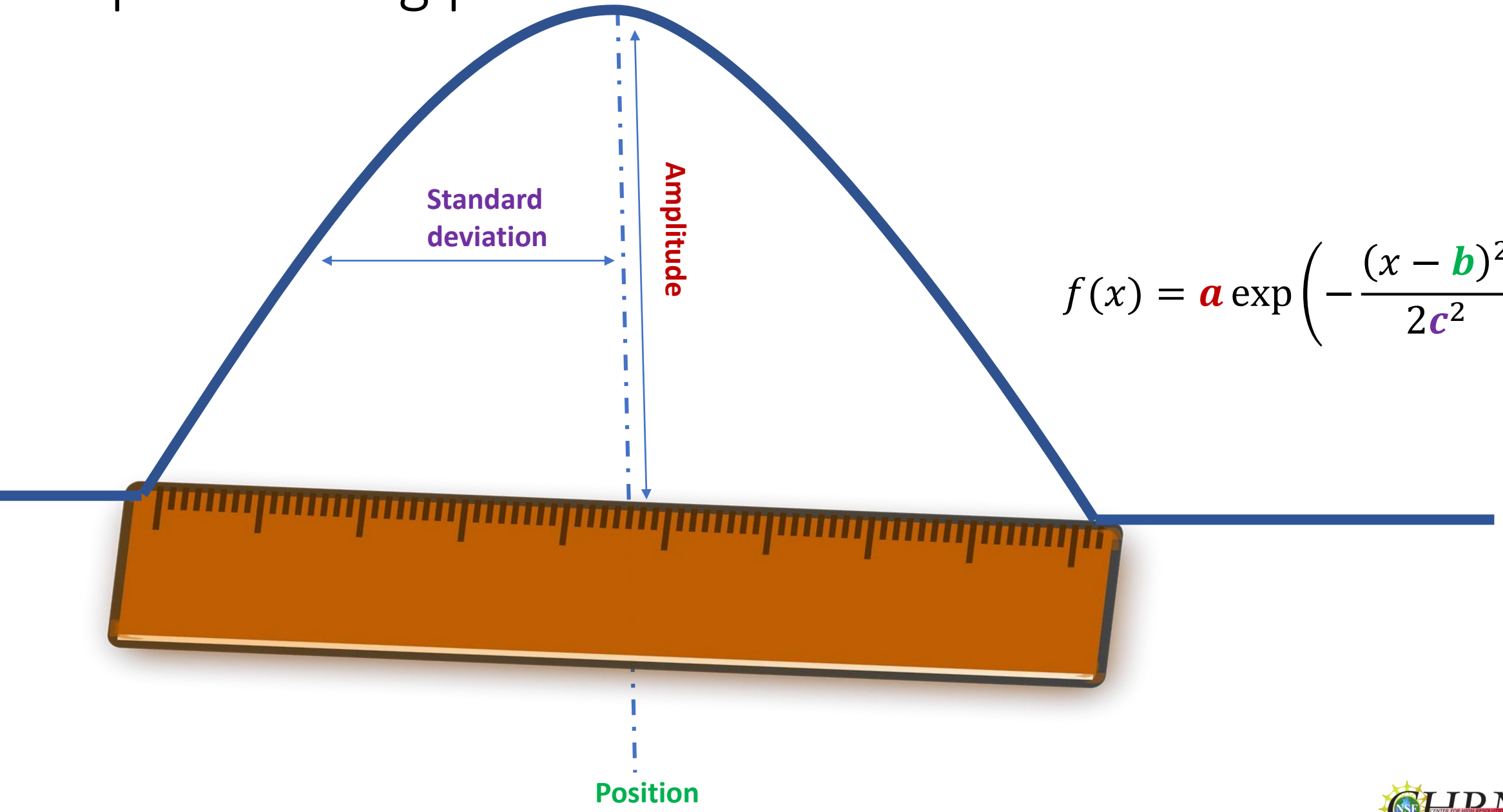


Two – step approach

1. Finding peaks

2. Mapping peaks from different diffraction patterns to each other

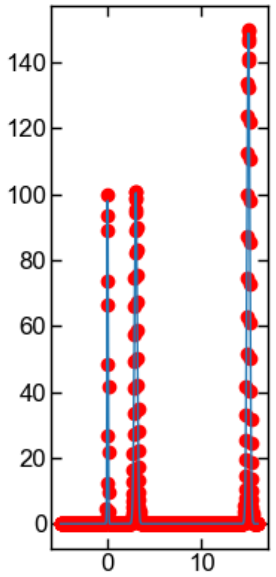
Step 1: Finding peaks

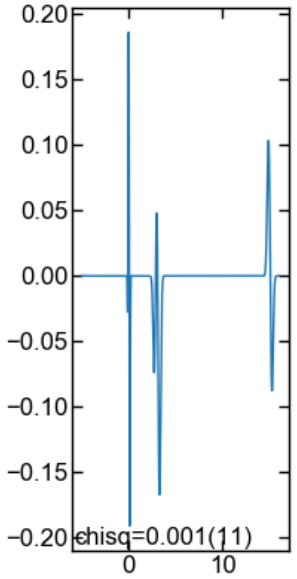


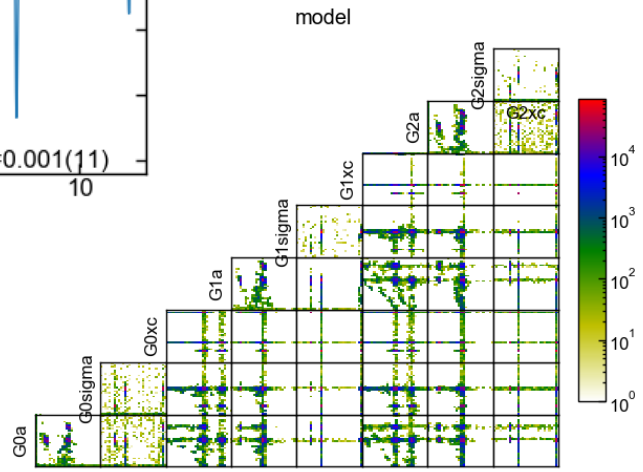
$$f(x) = \boldsymbol{a} \exp\left(-\frac{(x-\boldsymbol{b})^2}{2\boldsymbol{c}^2}\right)$$

Step 1: Finding peaks Bumps - DREAM

Software Package Developed by Paul Kienzle







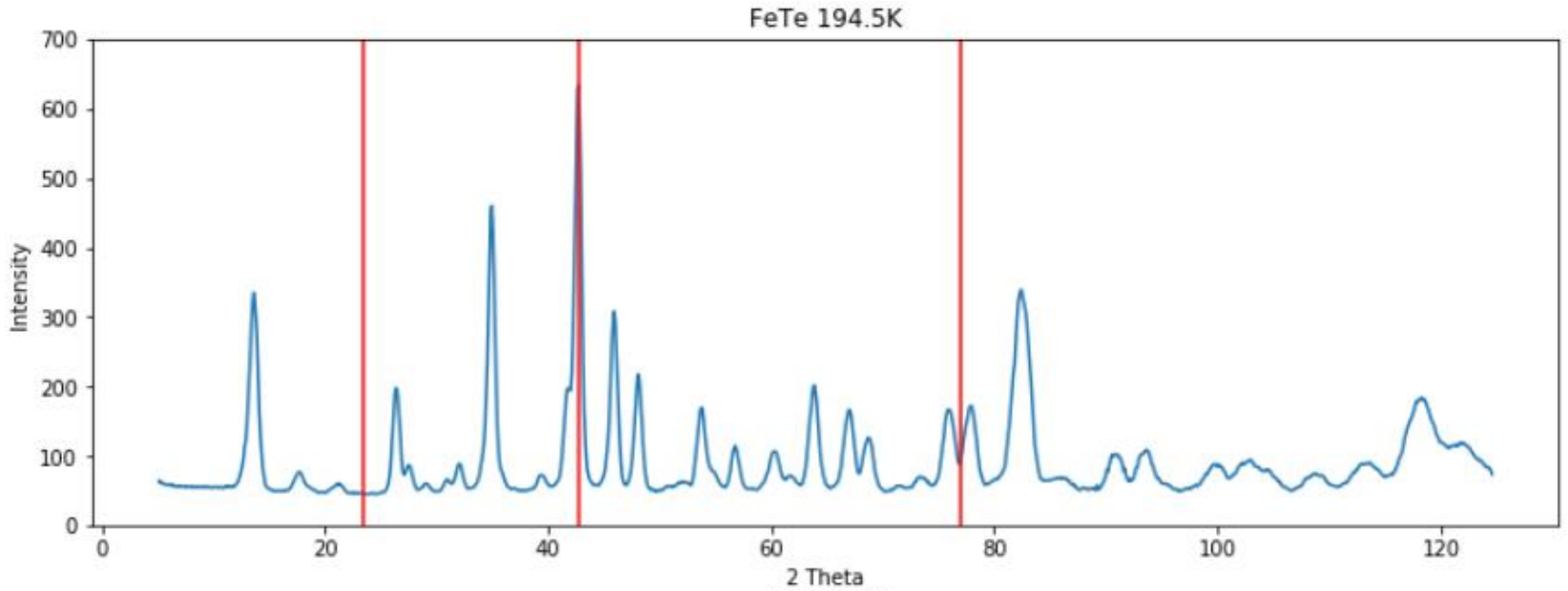
Actual parameters

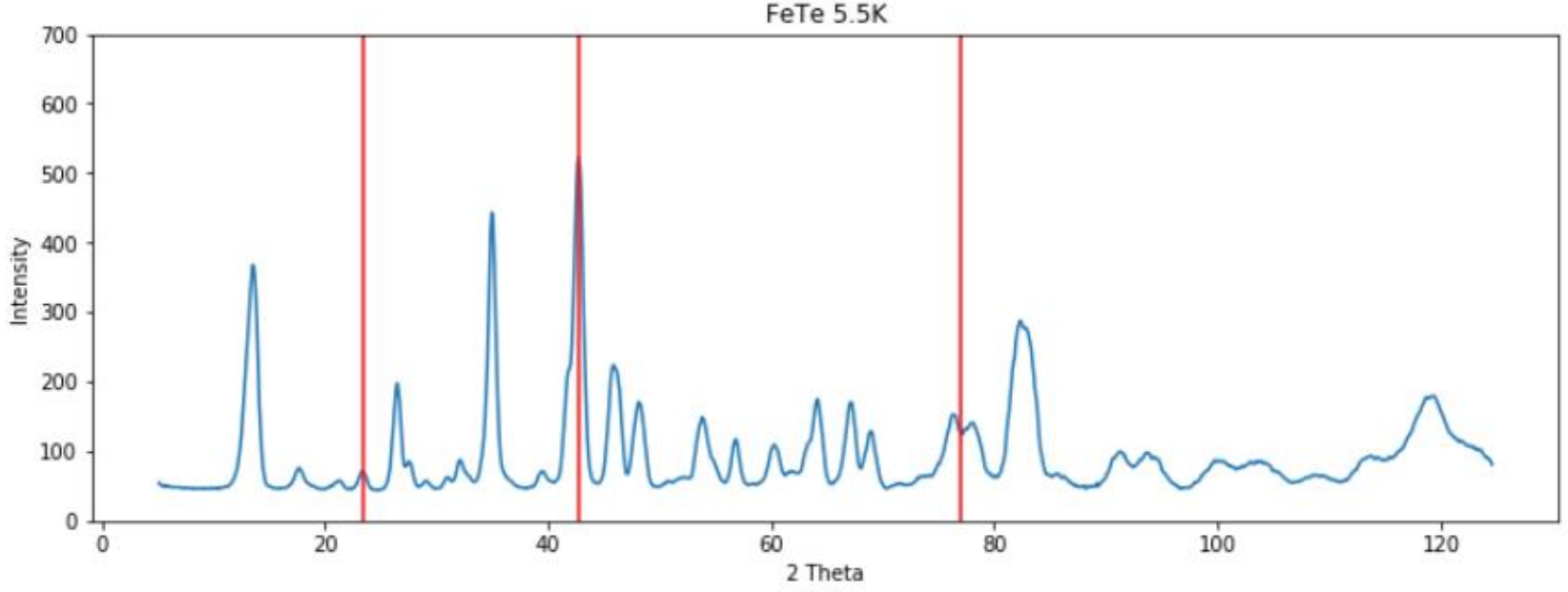
Amplitudes: 100, 150, 101

Positions: 0, 15, 3

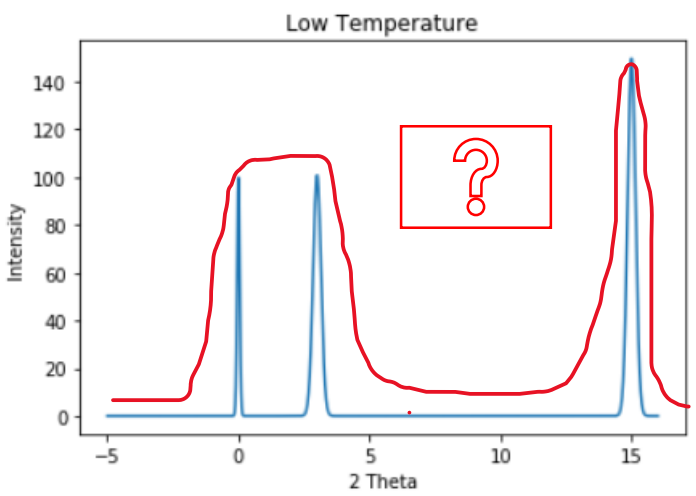
Standard Deviations: .05, .15, .15

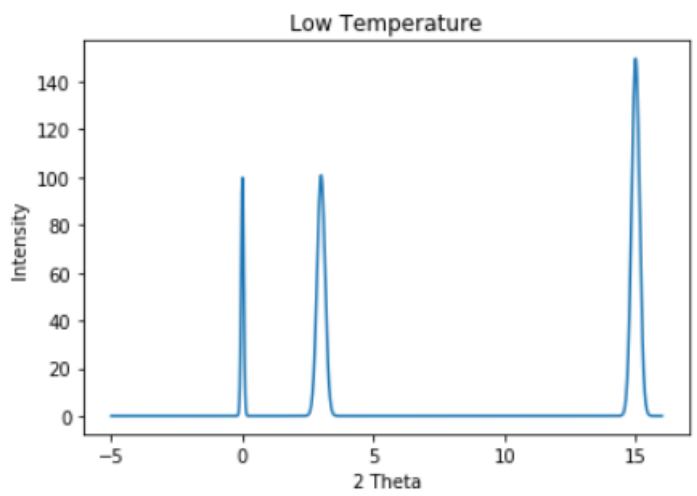
```
[0]
  .a = G0a = 149.17 in [0,200]
  .sigma = G0sigma = 0.150417 in [0,0.3]
  .xc = G0xc = 15.0015 in [-5,16]
[1]
  .a = G1a = 98.1573 in [0,200]
  .sigma = G1sigma = 0.050735 in [0,0.3]
  .xc = G1xc = 0.000934766 in [-5,16]
[2]
  .a = G2a = 100.542 in [0,200]
  .sigma = G2sigma = 0.151976 in [0,0.3]
  .xc = G2xc = 3.0013 in [-5,16]
```

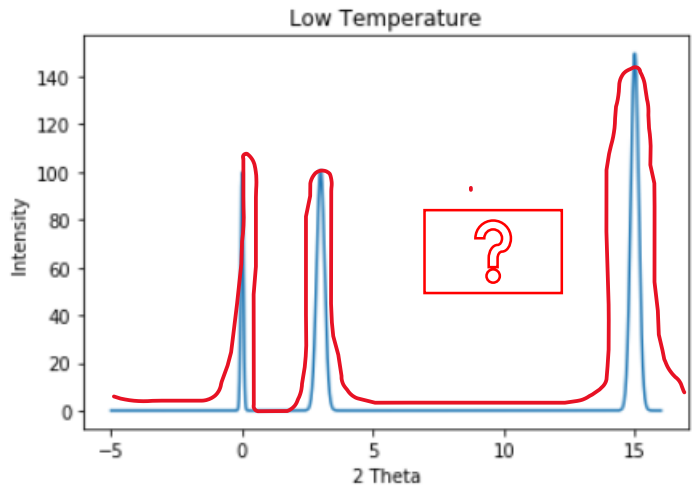

FeTe 194.5K
Intensity
2 Theta
0
100
200
300
400
500
600
700
0
20
40
60
80
100
120

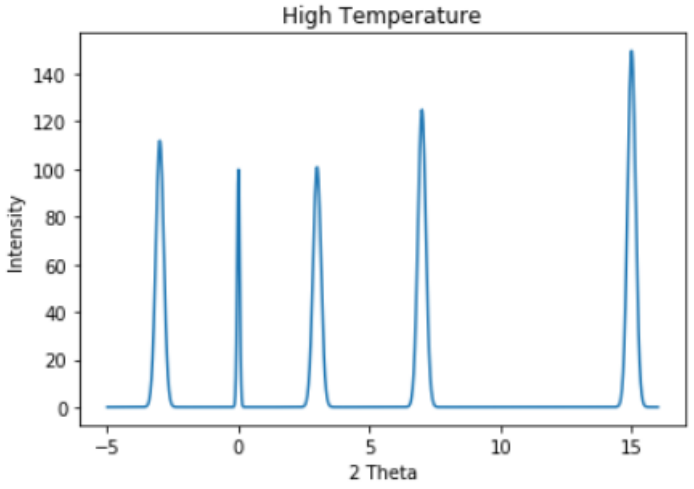

FeTe 5.5K
Intensity
2 Theta
0
100
200
300
400
500
600
700
0
20
40
60
80
100
120

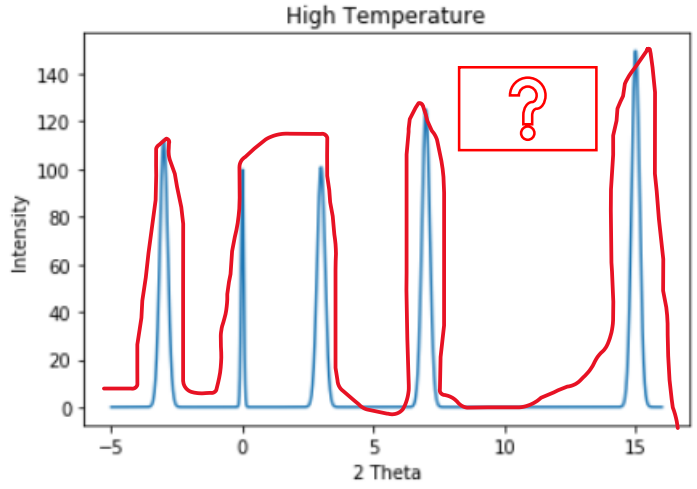
Step 1: Finding peaks

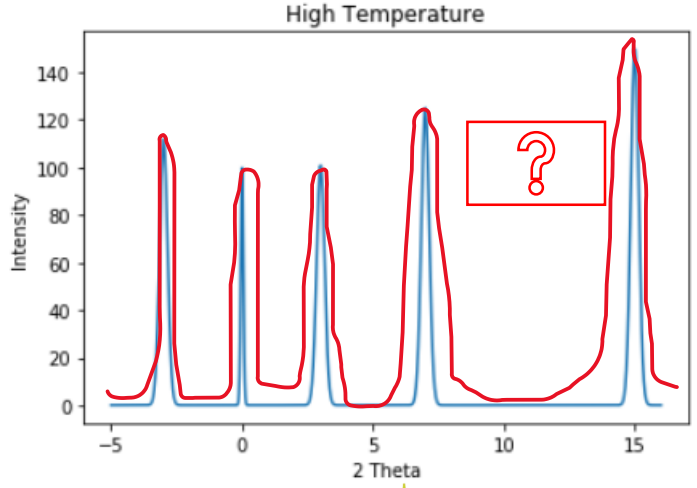










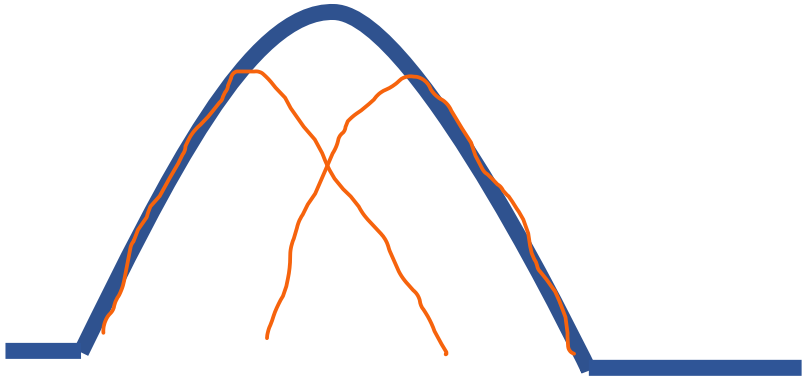


Step 1: Finding peaks
Bayesian Information Criterion (BIC)

$$\mathrm{BIC} = k\ln(n) - 2\ln(\widehat{L})$$

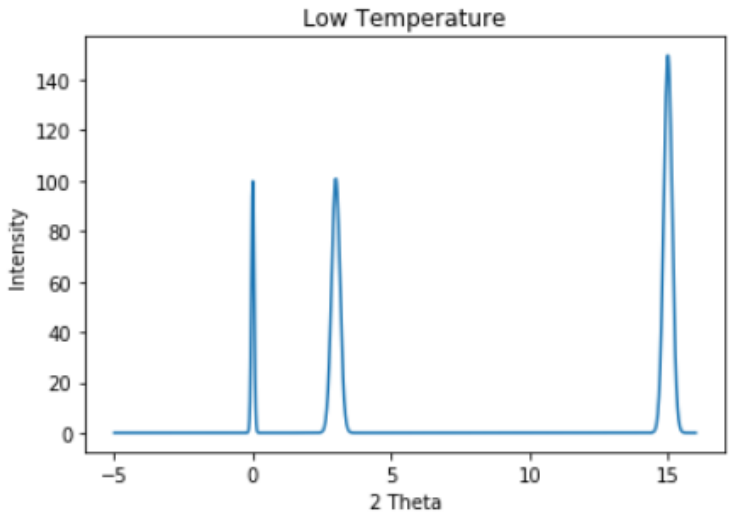
k = # of parameters n = number of data points L = maximum log-likelihood

$$\chi^2 = \left(\frac{1}{D.O.F}\right)\sum\frac{(O-E)^2}{E^2}$$

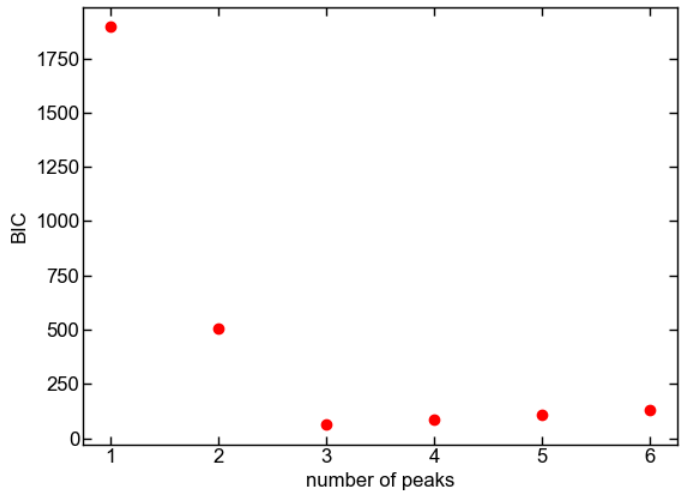


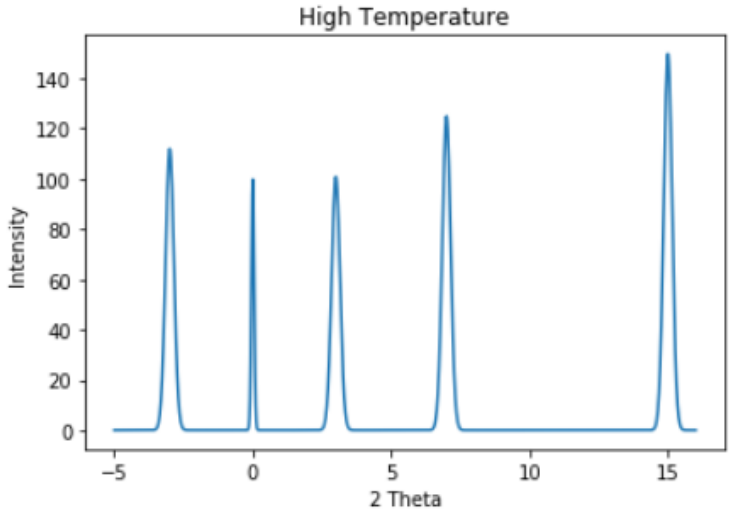
O = Observed data value
E = Expected data value
D.O.F = Degrees of Freedom

BIC plots

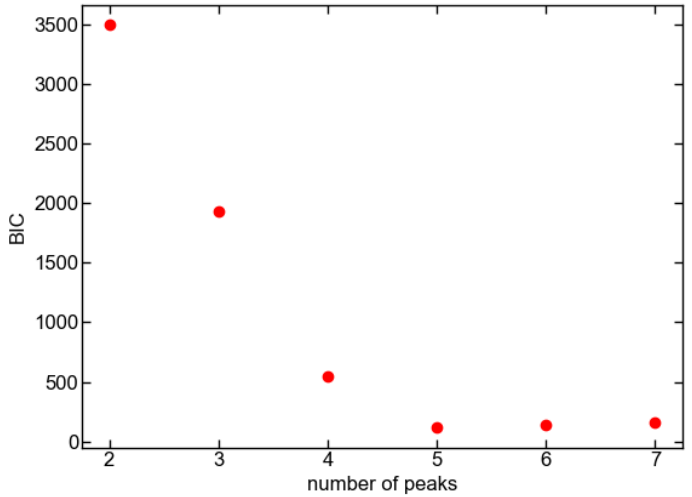


Low Temperature





High Temperature



Conclusions

- Fitting peaks first using probabilistic approach as opposed to mapping individual data points to each other directly seems more promising
- Summer Summary:
  - We used Bumps + DREAM to fit peaks to simulated data
  - We integrated code for automatically determining how many peaks to fit

In the process:

- Learned to use CLI, GitHub
- Gained familiarity with modules

Next Steps

- Testing on actual data/with more noise
- Improving Step 2 (Mapping)
- Generalizing from Powder to Crystal (1-D data to 2-D data)

Acknowledgements