Automated Discovery of Temperature Dependent Structural Change

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https://github.com/gcsantucci/SMC_DataChallenge17

1. Introduction and Data Inspection

In this study we look for phase transitions as a function of temperature by inspecting data from neutron diffraction experiments.

A phase transition is defined here as a structural change in the analyzed material.

The data is consists of curves of Intensity as a function of d-spacing for different values of temperature.

Figure 1 shows different Intensity curves for nine different values of temperature.

Figure 2 summarizes the curves for all temperatures.

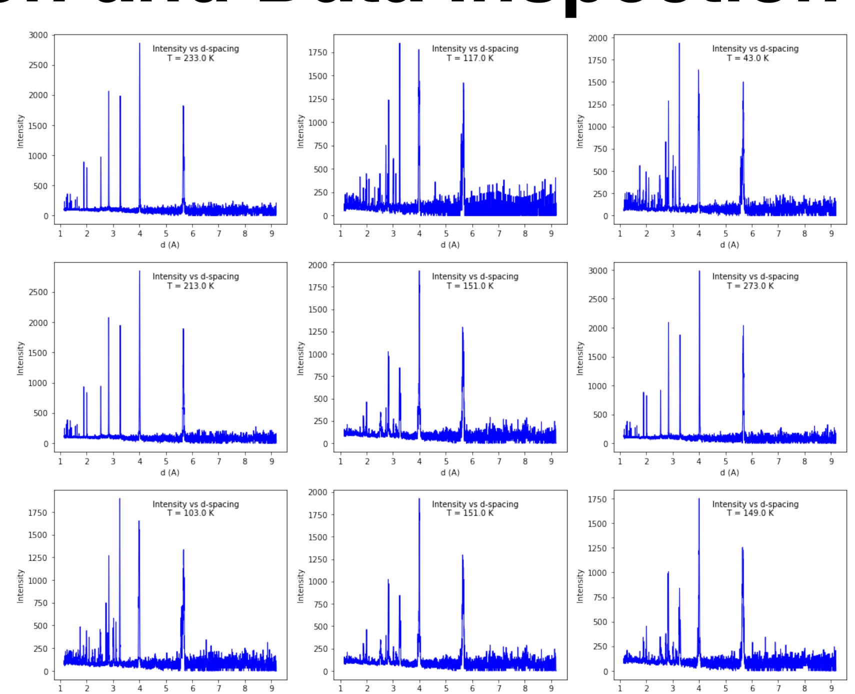

Fig. 1: Intensity curves for different values of temperatures.

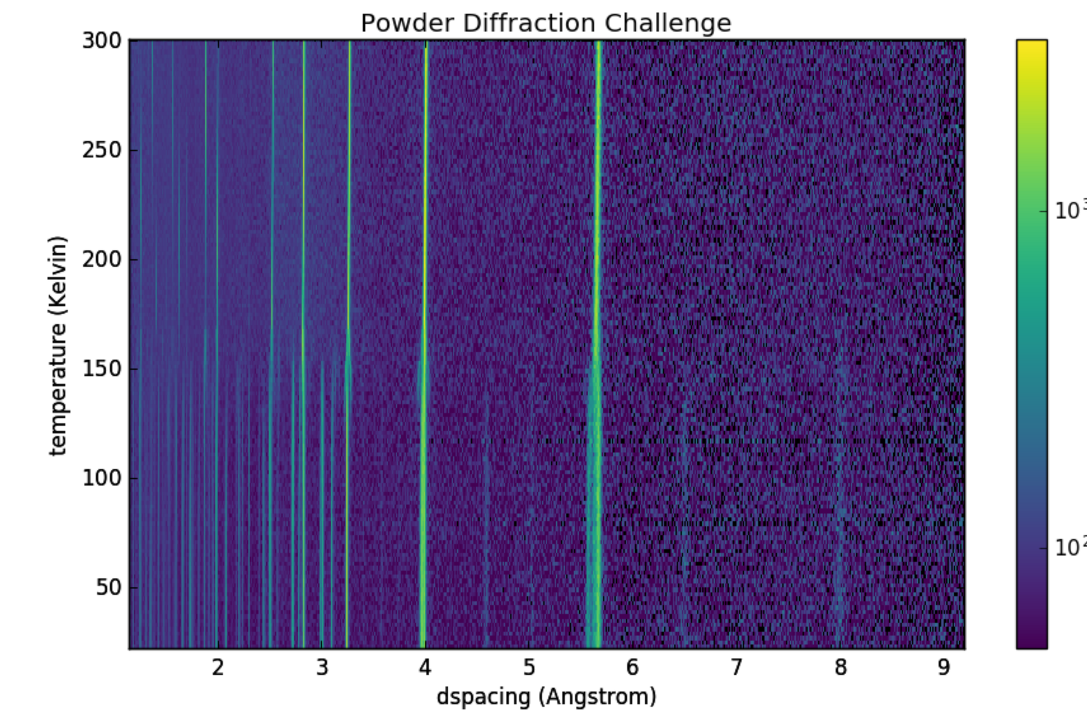

Fig. 2: Intensity (z) curves for all values of temperatures.

2. Finding the Phase Transition

To detect the temperature in which the phase transition occurred we look for the location in d-space of the highest intensity peak.

We can see that this location changes after a certain temperature - defined as the phase transition temperature (Figure 3 top).

To determine this temperature, we see where the difference between two consecutive locations is maximal (Figure 3 bottom).

$T_{phase} \equiv$ T where difference is maximal.

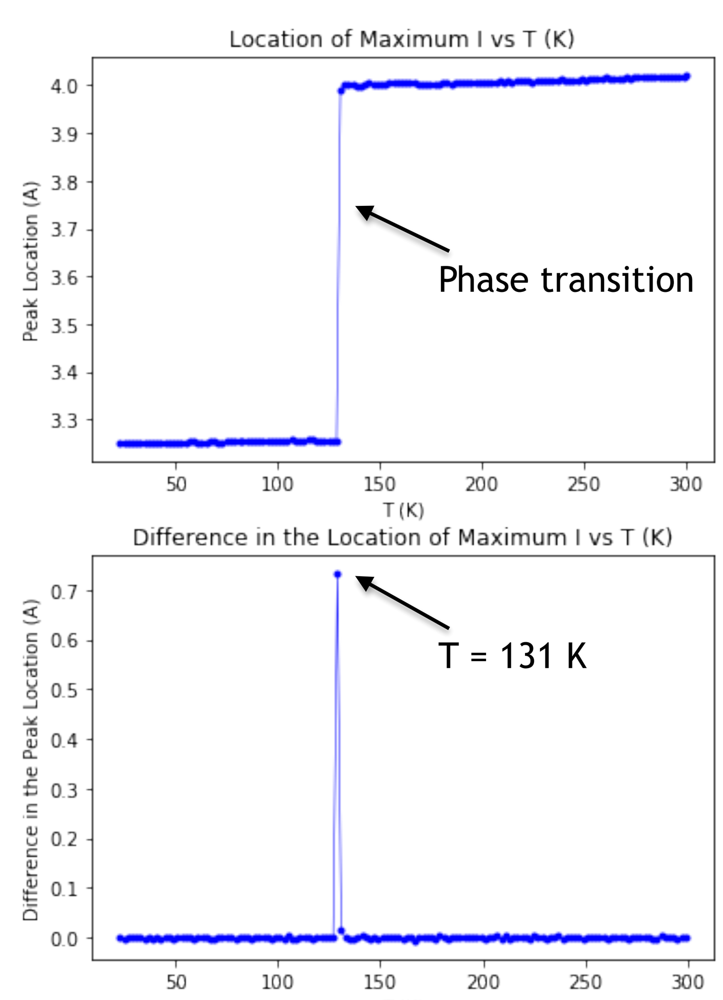

Fig. 3: Location of the Maximum Peak (top) and difference between consecutive temperatures (bottom).

3. Characterizing the 3.25 Å Peak

To characterize a peak we fit a gaussian plus background function centered in the location of the peak.

Figure 4 shows the results of the fit for two values of temperature, away (top) and close (bottom) to the phase transition.

We can see that close to the phase transition the peak is not gaussian at all. But since we are only interested in finding the phase transition and not the absolute values of Mean and Width, we can use the non-gaussianity to detect the phase transition.

Figure 5 shows the normalized values of Area, Mean and Width of the fit for all values of temperature.

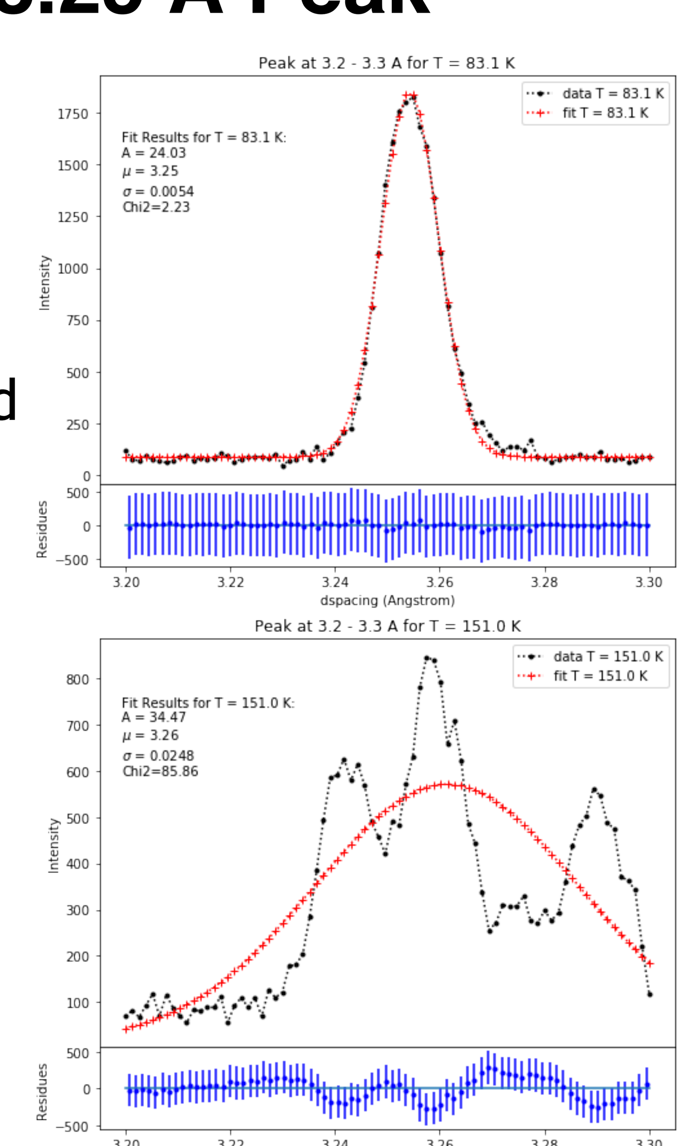

Fig. 4: Gaussian fit for T = 83 K (top) and T = 151 K (bottom).

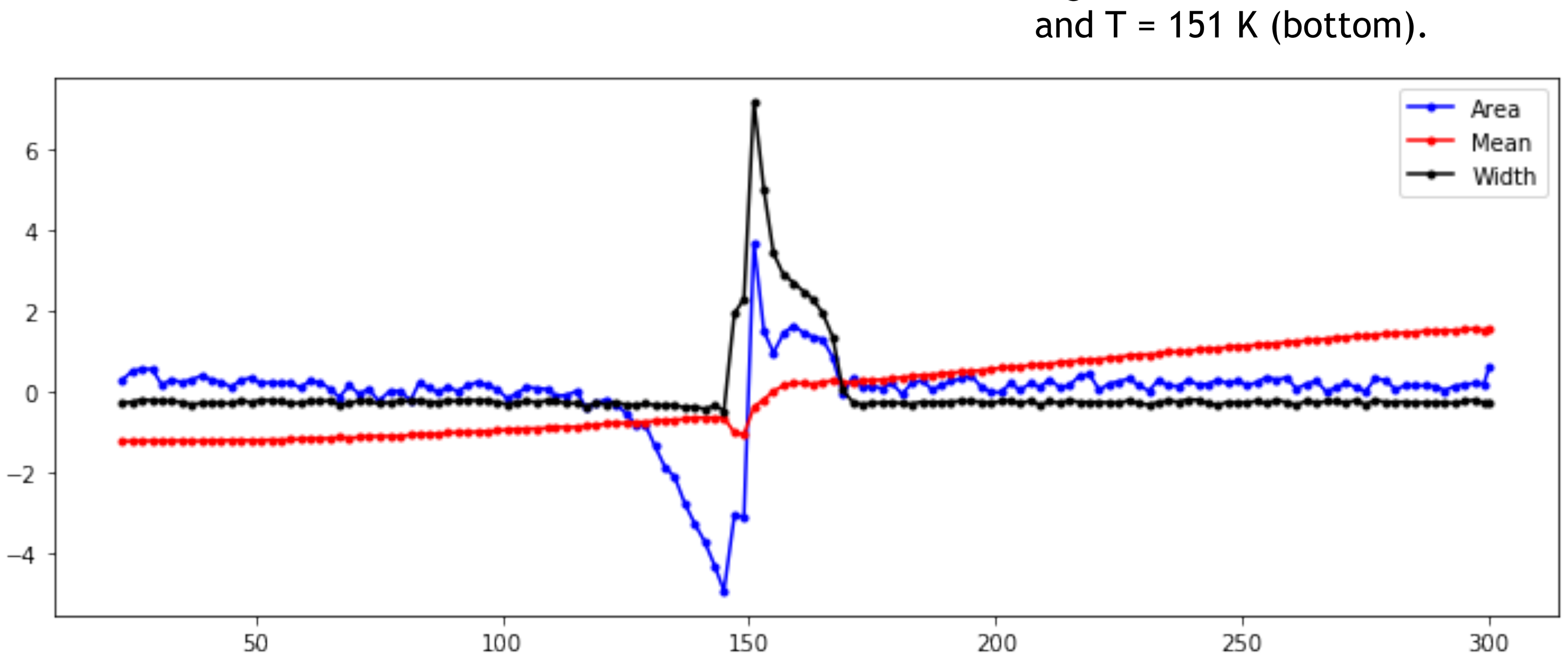

Fig. 5: Normalized Area, Mean and Width of the 3.25 A peak as a function of Temperature.

4. Peak Detection

To detect all the intensity peaks given a certain temperature we use the following algorithm:

- All the points are pseudo-peaks;
- Remove all points with height less than threshold - mph;
- Remove all peaks that are too closer to another peak - mpd;
- Promote the remaining pseudo-peaks to peaks and return a list.

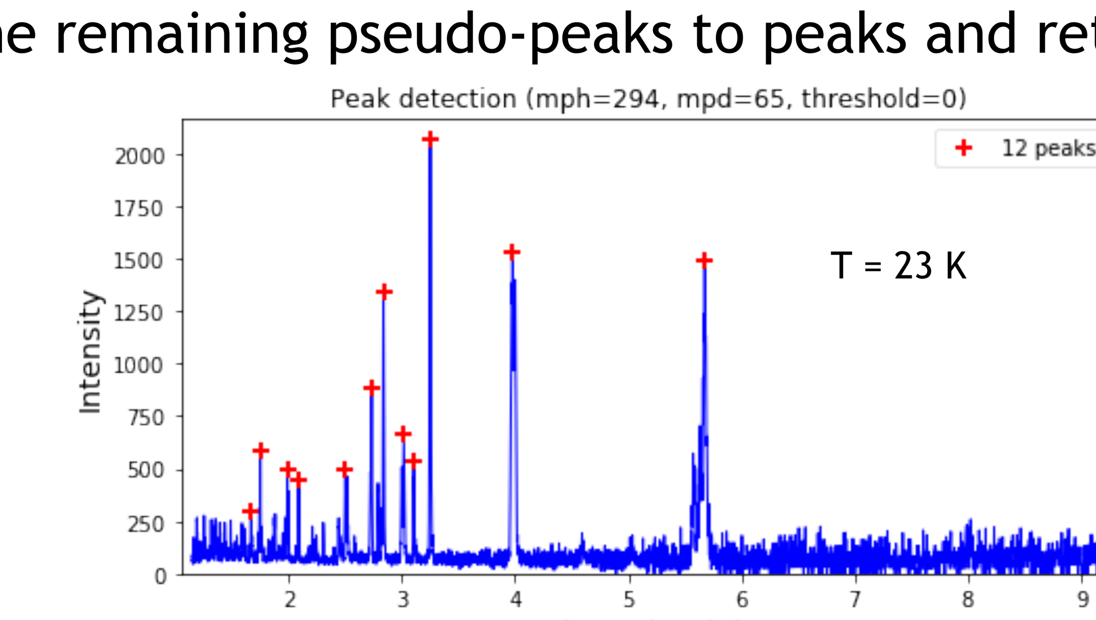

Fig. 6: Peak finding algorithm based on [1].

[1]: http://nbviewer.jupyter.org/github/demotu/BMC/blob/master/notebooks/DetectPeaks.ipynb

5. Characterizing All Peaks

Given two temperatures, we can get the list of centers using the peak detection algorithm. With these lists we can fit gaussians to all peaks as before and obtain a list of areas, Means and Widths for all peaks in both temperatures.

We define that a phase transition has occurred between the two temperatures if the mean of the 3.25 Å peak has shifted by more than 2 mÅ or if the width of this peak has changed by more than 1mÅ.

The average time to perform the presented analysis is safely below 5s since the analysis is very simple. The algorithm consists of finding all the peaks (simply removing values from a list) and performing a few gaussian fits.

Figure 7 shows the time the algorithm took for each pair of temperatures.

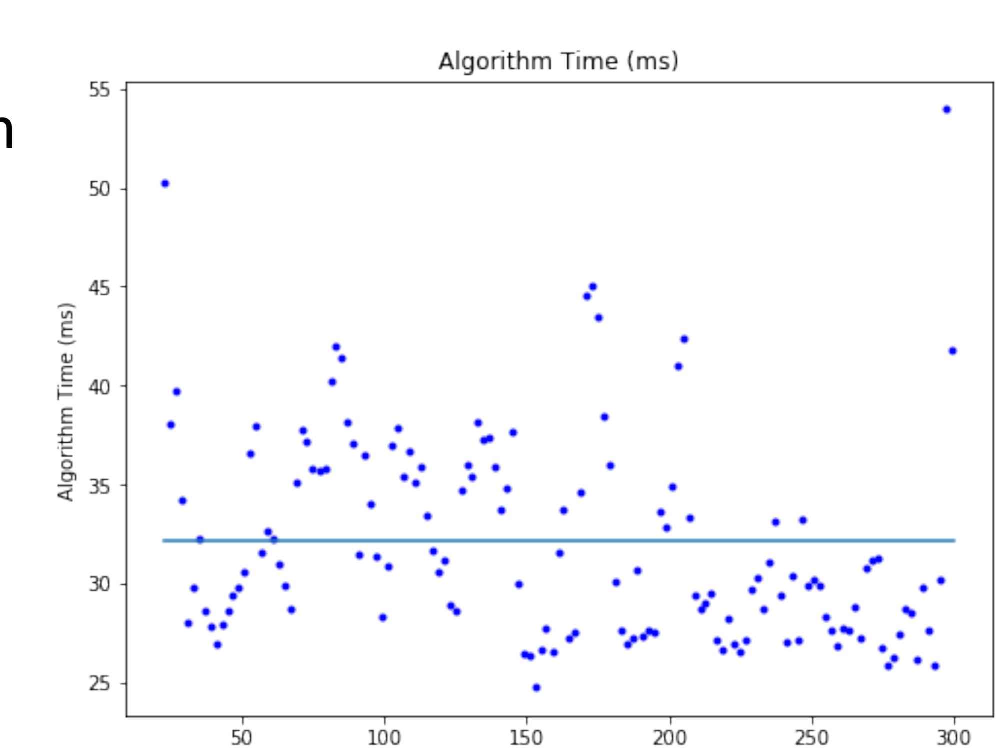

Fig. 7: Time of running the algorithm for each T.

6. Conclusions

In this work we presented a method for finding the temperature of a phase transition in a material using samples from neutron diffraction data.

We also explored the show how to characterize the intensity peaks in diffraction data and how to use them to detect a phase transition.