Each of 4 reflection fitting routines were constructed and tested using 5 data sets. Two of the filters had two variants and were tested with and without performing an autocorrelation prior to fitting. Two additional filters were tested from the previous software generation. This resulted in 14 variants. Each routine begins by isolating the individual reflections based on a percentage of the diffraction vector. The routines were:

- Paraboloid filter: This method fits a paraboloid to each reflection in the diffraction pattern.
- Ellipse filter: Same as the circle but fit an ellipse rather than a circle.
- Disk filter: Similar to the circle and ellipse filters however the fit is performed by fitting a circle to the reflection convex hull using a Nelder-Mead simplex minimizer.

The experiment was designed and statistically analyzed with the Design Of Experiment (DOE) methodology. This method is used to systematically investigate process variables that influence product quality. In this case the measure of product quality was the standard deviation of the strain in 002 and 220 directions. The results shown herein focus on determining the best reflection finding algorithm and the effect of the autocorrelation. Figure 5 shows the main effects plots for these results using the sensitivities of the [002] and [220] directions. The probability values for the tests related to determining the best peak fitting algorithm were 0.85 and 0.48 respectively for the data in the [002] and [220] directions. These values are well above 0.05 and are not statistically significant. Therefore, it was not possible to determine the best peak fitting algorithm with statistical significance. This result is further confirmed by the box plots shown in Figure 6. The fact that the box plots all overlap one and other demonstrate a lack of uniqueness and suggests that none are either much better or worse than the rest for the 5 datasets investigated. All data new algorithms performed better than the existing TC algorithm. The right side plots in figure 5 show a strong and almost identical effect of the autocorrelation on the data analyzed. This data shows that using the autocorrelation strongly influences the sensitivity of the data processed. The p-value for this effect was 0.003 in both directions. An autocorrelation has a strong and statistical significant positive effect (p-value must be < 0.05 to be significant).

Future work will focus on both better understanding the effect of the autocorrelation and the processing of diffraction data and on determining the best conditions for acquiring NBD data. The fitting routines will be analyzed both with and without the autocorrelation. These results will then be used to optimize the conditions for data acquisition.


References


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