Tutorial 1
X Ray Diffraction

Linda Crandall and Maggie Huff

July 10, 2017

Date Performed: July 7, 2017
Instructor: Chris Pratt

1 Objective

To get to know the diffractometer and X'Pert Data Collector, learn how to identify an unknown sample with X'Pert High Score software.

2 Results and Conclusions

Our 'unidentified' sample is silicon, which we ascertained after using the search peaks tool in the software. We eliminated the Kα_2 peaks, as well as peaks whose low intensity categorizes them as background. The program matches the peak pattern to ICDD known peak patterns and returns a match along with a score for how certain the match is.
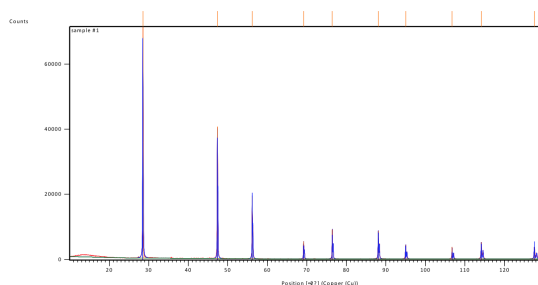

Figure 1: background cleaned peaks for sample overlaid with ICDD silicon peaks

Peak List: (Bookmark 3)

Pos. [°2θ]	Height [cts]	FWHM Left [°2θ]	d-spacing [Å]	Rel. Int. [%]
28.5179	72248.55	0.1378	3.13001	100.00
47.3783	40531.58	0.0960	1.91724	56.10
56.1835	19011.58	0.1200	1.63585	26.31
69.1850	5356.42	0.1200	1.35679	7.41
76.4496	9078.34	0.1200	1.24493	12.57
88.0846	8659.68	0.1440	1.10804	11.99
95.0133	4364.21	0.1440	1.04468	6.04
106.7627	3602.28	0.1440	0.95973	4.99
114.1449	5108.63	0.1680	0.91772	7.07
127.5840	3596.87	0.2160	0.85856	4.98

Pattern List: (Bookmark 4)

Visible	Ref. Code	Score	Compound Name	Displacement [°2Th.]	Scale Factor	Chemical Formula
*	00-027-1402	100	Silicon	0.059	0.942	Si

Figure 2: X'Pert HighScore also provides a peak list in the report

3 Discussion

Some considerations can help the use of X'Pert HighScore: choosing single phase over multi-phase, for instance, can influence the match automatically chosen by the software and thus the scores of each candidate for a match.

4 Answers to Multiple Choice Questions

(1) What information can you get from an ICDD file? d (Lattice parameters, crystal structure, and space group)

(2) When using X'Pert HighScore to analyze a sample, what feature is generally used in choosing a match? The search peaks feature, and the Analyze tool set. The program gives a candidate score, which we then use to choose a match.

(3) Why do we allow a pattern shift during a search match? Some x-ray diffraction machines are calibrated slightly differently than others, so a pattern shift allows for the absolute position of the peaks to change but their relative positions remain fixed.

(4) When you accept a pattern from the candidate list what happens to the rest of the candidates on the list? If you drag a candidate from the list up to the accepted area, that candidate's score is now higher and the rest of the candidates on the list get a lower score.

(5) If a pattern is automatically identified, is it guaranteed to be correct? No, especially if you have chosen the wrong phase or you have a complicated sample.

2

(6) What parameters can be changed to change the score of the candidates? Dragging a candidate up to accepted or deleting it from the list, possibly identifying the sample as a different phase.