

NEW FEATURES IN SIEve+, A PLUG-IN PROGRAM FOR PDF-4+/DDView+: HANAWALT, FINK AND LONG8 SEARCHES BASED ON REDUCED DATA AND NEW FULL PATTERN SEARCH/MATCH

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In an attempt to fill the gap between fully automated search/match programs and purely manual methods based on paper products, SIEve+ has been developed for extracting search/match information from the PDF-4+ powder diffraction databases [1,2]. The classical search algorithms are based on Hanawalt or Fink methods. The Hanawalt method is based on the d-spaces of the 3 strongest Bragg lines, whereas Fink is based on the 8 longest of the strong lines [2]. More recently, we have implemented a Long8 search that is related to Fink except that the intensity criteria is removed. These methods assume that if a suitable match is not found, then a rotation operator is used to permute the order of the d,I pairs and a subsequent analysis is performed. In this paper, we will show SIEve+ results that use automatic rotation operators to retrieve candidate hits from the PDF-4+ database. We continue to use the Goodness of Match (GOM) parameter to assess the quality of the search-indexing results. The objective of this enhanced analysis is to find the best candidate match between the unknown pattern and data in the PDF-4+ database.

In addition to the enhancements described above, we have also developed tools for total pattern matching. These have been integrated into SIEve+. In PDF-4+, we use on-the-fly technology to calculate digitized data for all entries in the PDF-4+. Thus, ~250,000 patterns are available. For search/match, the idea is to combine 3 independent tools: Boolean filters to locate candidate entries in the database, reduced pattern d,I pairs in search/match, and total pattern analyses to identify candidate matches from the digitized data in the database and the digitized experimental powder pattern. Walter, Hofmann and Kuleshova [3] have discussed a new similarity index for crystal structure determination from X-ray powder patterns. We have applied this formalism to total pattern matching, using SIEve+. In this formalism, a perfect total pattern match gives a similarity index, SI=0%; a complete mismatch has SI=100%. In this paper, we shall show results for Hanawalt/Fink Search-Indexing for which the GOM results do not yield clear phase identification results. However, when search/match is used in conjunction with the similarity index, proper phase identification is achieved. The conclusion we reach is that ambiguity in search/match results, from reduced d,I data, can be clarified using full pattern search/match methods.

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- [2] J. Faber, C. A. Weth and J. Bridge, *Powder Diffraction* **19**, 26-30 (2004).
- [3] D. Walter, M. Hofmann and L. Kuleshova, *J. Appl. Cryst.* **38**, 861-866 (2005).