

AUTOMATED ANALYSIS OF POWDER X-RAY DATA USING SCRIPTING AND DATA PIPELINING TECHNIQUES

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Unlocking the full information content of powder X-ray data is by no means trivial. Even a seemingly simple task, such as to determine whether two powder patterns represent the same chemical structure, can pose challenges as factors such as preferred orientation and particle size can introduce a significant degree of variability in the actual appearance of the recorded pattern. In such cases computational algorithms can help to account for this variability and facilitate the analysis. This presentation introduces a platform to automate the usage of these techniques based on a combination of scripting and data-pipelining technologies. The data-pipelining environment allows for the graphical capture of best practices in terms of repeatable workflows that can be applied to an arbitrarily large number of datasets. Benefits of this approach include standardization, convenient and consistent treatment of large volumes of data, and knowledge sharing. To illustrate this technology we first discuss general aspects such as data handling, visualization, and storage of powder patterns. Next we show how refinement and quantitative phase analysis tasks can easily be applied to large volumes of data. Finally we discuss how clustering of large datasets can be performed using a pattern based quantitative phase analysis technique.