

Non-negative Matrix Factorization in XRD/PDF Data Analysis

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We validated the use of the non-negative matrix factorization (NMF) technique for automatically extracting physically relevant components from X-ray diffraction (XRD) data and atomic pair-distribution function (PDF) data from time-series data such as in situ experiments. Utilizing the nature of the data, we developed a fast two-stage algorithm for highly efficient and accurate NMF. In its second stage, an interior point method is adopted to accelerate the local convergence. Afterwards, in order to study data collected at different temperatures where the materials are undergoing thermal expansion, we extended NMF by introducing a new variable, the stretching factor, to describe any expansion of the signal. A further enhancement for the case of XRD data from crystalline materials was also proposed. When applied to real data from in situ chemical reaction experiments, it has been demonstrated to be successful.

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