BAYESIAN STATISTICS APPLIED TO THE RIETVELD METHOD

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A quantitative phase fraction, lattice constant and crystal structure refinement is frequently carried out by means of the Rietveld method. Coherent diffraction length and microstrain can e.g. be deduced by the double Voigt approach. Optimized model parameters are usually obtained by a least square algorithm. However, it is not guaranteed that the global minimum is found by this method when scanning the parameter space. This problem is circumvented by using a global optimization procedure, e.g. Bayes approach with a Markov Chain Monte Carlo (MCMC) algorithm. As a result of this MCMC algorithm not only the global minimum is detected but also probability distributions and correlations of the parameters are revealed. The Rietveld approach combined with the Bayesian statistics is applied to evaluate diffraction patterns of in situ high-temperature X-ray experiments. It has been observed that in contrast to the classical local minimization techniques acceptable results are obtained by means of Rietveld combined with Bayesian statistics even if the signal-to-noise ratio is low. As one of the future goals of this research work numerically stable, highly automated Rietveld algorithms should be established for industrial applications.