

Alternative Methods for Process Control in Aluminium Industries - XRD in Combination with PLSR

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Abstract

X-ray diffraction (XRD) is a standard tool for process control in aluminium industries. Varying raw material qualities, the use of different fluxes and increasing prices require a better control of processes and a more efficient use of energy. Traditionally quality control of electrolytic baths, alumina and bauxites has relied on calibration based single peak methods or more advanced full pattern techniques. A common method is the Rietveld quantification which uses structural information to predict information from the full pattern using physical models and fitting techniques. Sometimes this approach is stretched to its limits, especially when no realistic physical model is available, or when the model is either too complex or does not fit to reality. In such cases there is an elegant alternative: multivariate statistics and **Partial Least-Squares Regression (PLSR)**, a method that does not require pure phases, crystal structures or complex modelling of peak shapes. This paper describes the advantages of using PLSR and shows new results for the determination of electrolytic baths and bauxite directly from the XRD pattern.

Keywords: XRD; PLSR; electrolytic bath; bauxite; process control; X-ray diffraction.