A new method for quantitative phase analysis of multi-component polycrystalline materials using observed integrated intensities and chemical compositional data of individual crystalline phases

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Identification and subsequent quantification of individual crystalline phases in multi-component polycrystalline materials using X-ray powder diffraction technique are a first step for characterizing materials in research, development and production. The Rietveld and RIR (Reference Intensity Ratio) methods have widely been used as prompt analysis techniques for quantitative phase analysis (QPA). The former uses the structural information of individual phases and the latter uses observed and/or calculated RIR's for relating the weight fractions of individual phases with observed diffracted intensities. A new method proposed here has theoretically been derived, and it uses sets of observed integrated intensities and chemical compositional data of individual phases [Toraya, H. (2016). *J. Appl. Cryst.*, **49**, 1508 – 1516]. Two kinds of information can be derived from individual chemical formulae. One is the molecular weight, and it can directly be related with the weight of the relevant phase. The other is the numbers of electrons belonging to individual atoms in the formula, and it is used for incorporating the differences in scattering power among the relevant phases. Since the present method does not use the crystallographic information but just the chemical information, it can be applied to materials, for which no structural data nor RIR data are available, as well as those analyzed by current QPA techniques. Theory, test results and examples of practical applications will be discussed in the present report.