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Principal component scores projection on a barycentric coordinate system for a quantification in polycrystalline mixtures XRPD data without crystal structure data

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X-ray diffraction from powders is one of the most widespread techniques for the qualitative and quantitative analysis of polycrystalline mixtures and solid materials in general. In many cases, traditional methods fail to overcome intrinsic problems of the samples being analyzed (enhanced micro absorption and preferred orientations) or even just sample preparation (little sample, not homogeneous, little ground). Moreover, most traditional quantification methods require the knowledge of the crystal structure or at least pure phase XRPD profile only. In the last decade, several solutions based on multivariate statistical analysis have taken hold, on principal component analysis (PCA) [1]. This technique can limit the contribution of the experimental error contained in the data, to extract efficiently the useful information. However, PCA-based quantification passes through the construction of regression models, as happens for traditional methods based on internal standards. A novel method is proposed for the quantification of components in polycrystalline mixtures by X-ray diffraction data from powders, in principle without any a priori knowledge about crystal structure and/or pure phase profile. The method is based on a coordinate change proposed by Cornell in his book "Experiments with Mixtures" [2] and is virtually scalable for polycrystalline systems with any number of components. The mathematical methods are accompanied by two case studies recently published [3-4] to provide tangible examples of how the coordinate change method works in phase quantification. The results show that the developed method is fast and suitable for direct semi-quantitative analysis with no a priori structure information, which can be combined with a finer quantitative analysis, if necessary. The developed algorithm is presented in its form which has recently been integrated into RootProf [5], a software dedicated to X-ray diffraction data analysis.

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Primary author: Dr LOPRESTI, Mattia (Dipartimento di Scienze ed Innovazione Tecnologica, Università degli studi del Piemonte Orientale "Amedeo Avogadro")

Co-authors: Dr CALIANDRO, Rocco (Istituto di Cristallografia, CNR); Prof. MILANESIO, Marco (Dipartimento di Scienze ed Innovazione Tecnologica, Università degli studi del Piemonte Orientale "Amedeo Avogadro"); Dr PALIN, Luca (Dipartimento di Scienze ed Innovazione Tecnologica, Università degli studi del Piemonte Orientale "Amedeo Avogadro"); MANGOLINI, Beatrice (Cold Car S.p.A.,)

Presenter: Dr LOPRESTI, Mattia (Dipartimento di Scienze ed Innovazione Tecnologica, Università degli studi del Piemonte Orientale "Amedeo Avogadro")

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