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Quantitative phase analysis of polymorphs using only observed integrated intensities

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A new method for quantitative phase analysis of multi-component mixtures using a conventional-type X-ray powder diffractometer has been proposed [1]. A formula for quantification can derive weight fractions of individual crystalline phases from sets of observed integrated intensities measured in a wide 2θ-range, chemical formula weights and sums of squared numbers of electrons belonging to atoms in respective chemical formula units. The formula has been tested using several test samples, and it was demonstrated that the accuracy in derived weight fractions was well comparable to that by the Rietveld method [2]. The present method can be applied to any multi-component crystalline materials. When target component materials are polytypes or polymorphs, having the same chemical composition, however, the chemical formula weights and the numbers of electrons will fall off from the formula. Therefore, their weight fractions can be derived only from the observed integrated intensities and without using any structural knowledge nor chemical data of individual phases. What we do in practice is to observe integrated intensities of individual diffraction lines and to identify to which phase they are belonging. In research and development of new materials, such as of pharmaceuticals, new polymorphs are often found among the known polymorphs on X-ray powder diffraction pattern. X-ray analysis using the present method will give the information of relative quantities of polymorphs in the sample ahead of the other analytical techniques.

[1] Toraya, H. (2016). J. Appl. Cryst. 49, 1508 – 1516.
[2] Rietveld, H. M. (1969). J. Appl. Cryst. 2, 65 – 71.

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