Application Note B-XRD1115

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B-XRD1115 - Quantitative analysis of γ-Al_2O_3 by the DD method

Introduction

In quantitative analysis by the X-ray diffraction method, it is necessary to accurately determine the integrated intensities of peaks corresponding to each component. However, it is difficult to calculate integrated intensities for a compound having low crystallinity and, therefore, broad peaks. Our new quantitative analysis method, the Direct Derivation (DD) method, performs Whole Powder Pattern Fitting (WPPF) based on the measured profiles of a single component. As a result, WPPF can be easily performed even on compounds that show complex patterns that conventionally make it difficult to calculate the profile function from the crystal structure. Here, mixtures of α-Al_2O_3 and γ-Al_2O_3 were quantified.

Measurements and results

Al_2O_3 has polymorphic forms, α-type (high-temperature type) with high crystallinity and γ-type (low-temperature type) with low crystallinity. Here, three α-Al_2O_3 / γ-Al_2O_3 mixtures were created with α-Al_2O_3 concentrations of 1, 10 and 30 mass% respectively. The 2θ range from 5 to 120° was measured at 10°/ min. Figure 1 shows the obtained X-ray diffraction profiles in multiplex format, and Table 1 shows the R_{wp}, S value, preparation value and quantitative value of the analysis results of the three mixtures. The results show that accurate quantitative values can be calculated for substances with low crystallinity.

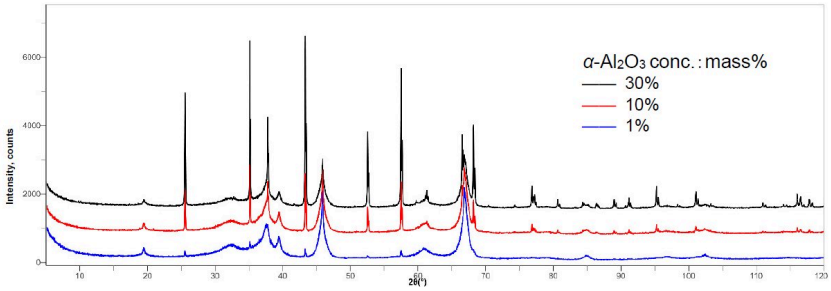

Figure 1: Multiple X-ray diffraction profiles obtained from mixtures of α-Al_2O_3 and γ-Al_2O_3

Table 1: R_{wp}, S value, preparation value and quantitative value for α-Al_2O_3 (mass%)

	1%	10%	30%
R_{wp} (%)	8.58	7.70	7.69
S	1.3188	1.1698	1.1527
Preparation value	1.01	10.01	30.04

Quantitative value	1.01(3)	9.96(4)	29.67(4)

References

(1) H. Toraya: *J. Appl. Cryst.*, **49** (2016) 1508-1516.
(2) H. Toraya: *J. Appl. Cryst.*, **52** (2019) 520–531.

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