Application Note B-XRD1127

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B-XRD1127 - Background reduction for iron oxide with CuKa X-rays using XRF mode

Introduction

A Cu target is widely used for X-ray diffraction measurements because it efficiently generates X-rays due to its excellent thermal conductivity and is inexpensive. Additionally, the wavelength of the characteristic line Kα1 allows observation up to a d-value of 0.82 Å (2θ = 140°), so it is suitable for determining crystal structures at atomic position level. Despite these advantages, diffraction profiles for Fe compounds exhibit high backgrounds due to fluorescent X-rays generated by Fe, which makes it difficult to distinguish low-intensity diffraction peaks from the background. Here, we illustrate diffraction results with low background and a high P/B ratio obtained using the X-ray fluorescence reduction mode of a 2D detector with a Cu source.

Measurements and results

Figure 1 shows the diffraction profiles of iron(III) oxide observed using Cu and Co sources, two detectors (D/teX and HyPix-400), and different energy modes (standard (Std) and X-ray fluorescence reduction (XRF)) (a), and the profiles normalized by the background (b). The ratios of peak intensity (P) and background (B) of the main peak ($Q \approx 2.3$ Å^{-1}) of iron oxide are shown in Table 1. The backgrounds using Std mode of D/teX and HyPix-400 with a Cu source are higher than those using Std mode of those detectors with a Co source due to the generation of fluorescent X-rays by the Fe atoms. However, the P/B ratio with a Cu source improves by a factor of 9 compared to the Std mode of D/teX and 39 times compared to the HyPix-400 when the detector is operated in XRF mode. In addition, the results for XRF mode of HyPix-400 with a Cu source are approximately 8 times better than with the Std mode of HyPix-400 with a Co source. As described above, even with a sample containing iron, diffraction profiles with low background and high P/B ratio can be obtained using the XRF mode of HyPix-400 without changing the Cu target.

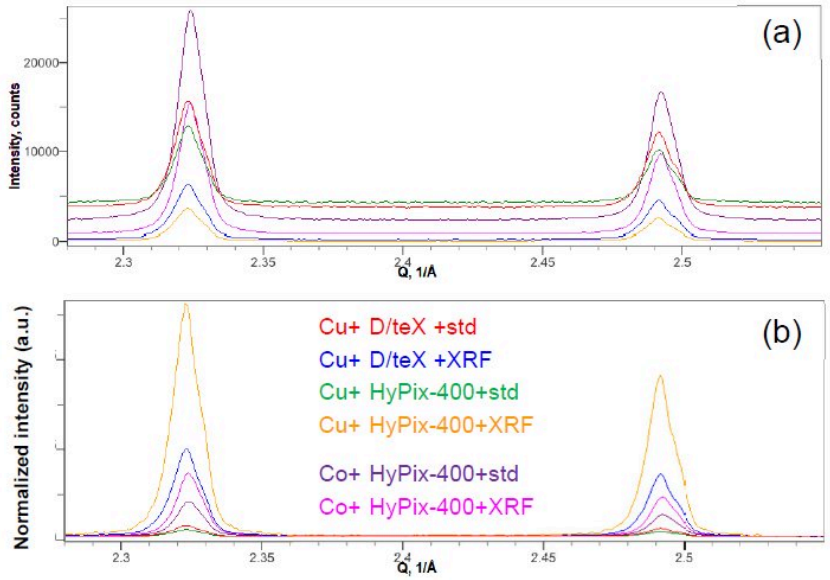

Figure 1: The observed diffraction profiles (a) and normalized profiles (b) of Fe_2O_3 by Cu and Co sources, detector types, and their energy modes (Std: standard mode, XRF: X-ray fluorescence reduction mode).

Table 1. Peak(P)-to-background(B) ratio of the main peak (Q ≈ 2.3Å^{-1}) of Fe_2O_3

X-ray	Detector	Energy mode	P	B	P/B
Cu	D/teX	Std	12131	3723	3
		XRF	6076	224	27
	HyPix-400	Xtd	8655	4281	2
		XRF	3606	46	78
Co	HyPix-400	Xtd	23688	2265	10
		XRF	14559	751	19

Related products

HyPix-3000

Compact photon counting x-ray detector

MiniFlex

New sixth-generation general purpose benchtop XRD system for phase i.d and phase quantification