Powder diffraction optics for SmartLab X-ray diffractometer

1. Introduction

Rigaku SmartLab is a multipurpose, fully-automated horizontal X-ray diffractometer that allows many types of measurements and evaluations of materials ranging from powders to thin films. Rigaku's expansion system and Cross Beam Optics (CBO) system enable configuration of a wide range of optics, while the SmartLab Guidance control software permits easy switching between optics for added versatility.

The many optics systems offered by Rigaku for SmartLab include CBO system incorporating a parabolic multilayer mirror, CBO-E system incorporating an elliptical multilayer mirror, and optics configured with the Kα1 unit with a Johansson Ge crystal for monochromatization of incident X-rays to the Kα1, designed to measure powder samples. These systems allow the user to configure the ideal optics for specific measurement or evaluation purposes. The new and unique Kα1 system enables various types of measurement while maintaining samples in a horizontal position.

2. CBO system

The optics of the CBO system permits easy switching of incident X-rays by simply changing the selection slit. Two systems are available: The CBO (Fig. 1) lets the user select the Bragg-Brentano focusing method or parallel beam method using a parabolic multilayer mirror, while the CBO-E (Fig. 2) lets the user select the Bragg-Brentano focusing method or convergent beam method using an elliptical multilayer mirror.

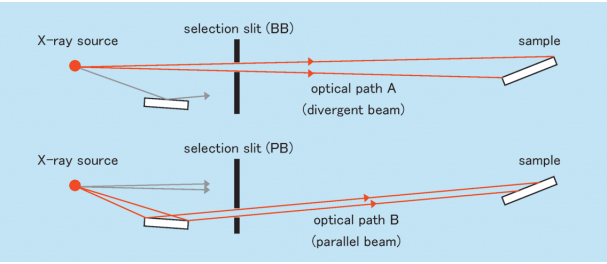

Fig. 1. Schematic diagram of CBO.

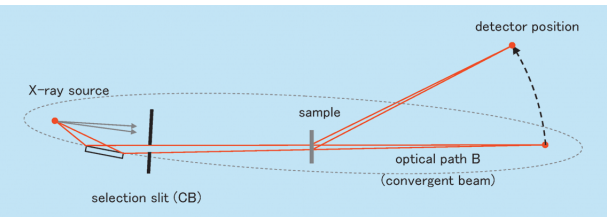

Fig. 2. Schematic diagram of CBO-E.

2.1 Bragg-Brentano optics

The Bragg-Brentano optics enables easy acquisition of high resolution and high intensity data by the reflection method (Fig. 3). It is generally used for qualitative and quantitative analysis of powder samples.

2.2 Parallel beam optics

The parallel beam optics allows accurate measurement of diffracted X-ray positions unaffected by sample shape (Fig. 4). It is generally used to analyze powder sample profiles and measure the degree of preferred orientation, as well as to measure thin-film samples.

2.3 Convergent beam optics

The convergent beam optics enables high resolution measurements by the transmission method (Fig. 5). It is used to measure samples with low absorption

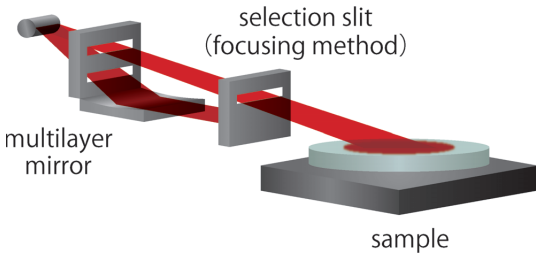

Fig. 3. Schematic diagram of CBO Bragg-Brentano optics.

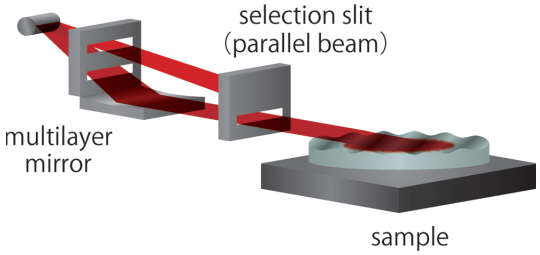

Fig. 4. Schematic diagram of CBO parallel beam optics.

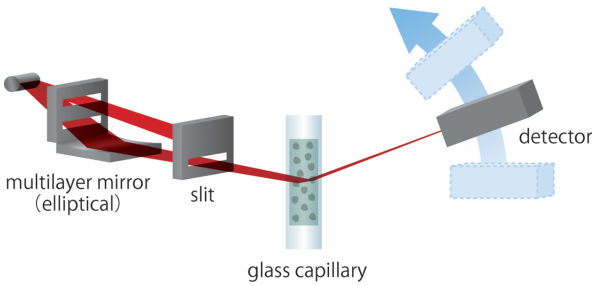

Fig. 5. Schematic diagram of CBO-E convergent beam optics.

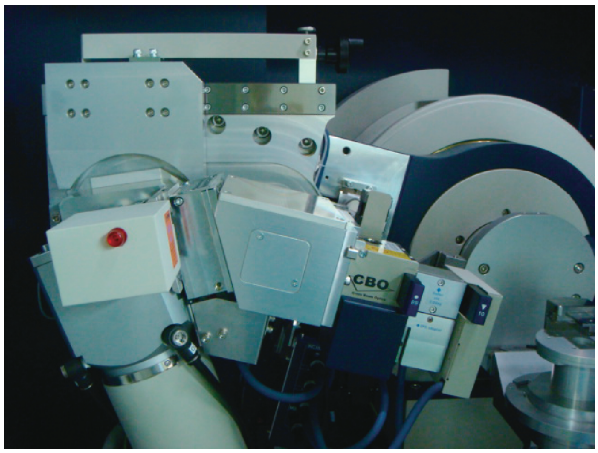

Fig. 6. Kα1 unit.

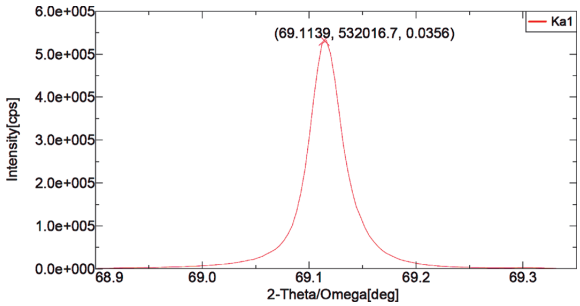

Fig. 7. Profile of Kα1 optics (Si (4 0 0)).

coefficients and preferred orientation, such as pharmaceuticals. Diffracted X-rays are focused on the detector surface for efficient measurement when combined with the D/teX Ultra 1D high-speed detector.

3. Kα1 system

Rigaku's expansion system also enables to install the Kα1 unit (Fig. 6). The user can easily switch between the conventional Kα and new Kα1 optics by installing/removing the Kα1 unit. Either of the optics can be selected depending on the purpose of measurements using your SmartLab.

Since incident X-rays are monochromatized to Kα1, even overlapped diffraction peaks can easily be decomposed. The peak positions, widths, and intensities will be determined more precisely in the diffraction patterns obtained using the Kα1 optics than using the conventional Kα1 optics. The Kα1 unit is recommended to be used for indexing or *ab initio* structure analysis, which requires high-resolution data.

4. Kα1 system+CBO system

The Kα1 system incorporates a Johansson Ge crystal for monochromatization. To allow use of the CBO system without modification, the focus position of the Kα1 system is designed to align with the conventional focus position. Simply by changing the selection slit, the user can direct X-rays monochromatized to Kα1 (Fig. 7) to Bragg-Brentano optics (Fig. 8), parallel beam optics (Fig. 9), or convergent beam optics (Fig. 10).

X-rays monochromatized to Kα1 can be used with the Bragg-Brentano focusing method and convergent beam method whereby diffracted X-rays are focused on the detector surface for efficient measurement when combined with the D/teX Ultra 1D high-speed detector. Compared to conventional monochromatization methods, this achieves faster high intensity measurements. Pairing the Kα1 unit with the CBO system lets users configure the ideal optics for the specific purpose of a measurement or analysis.

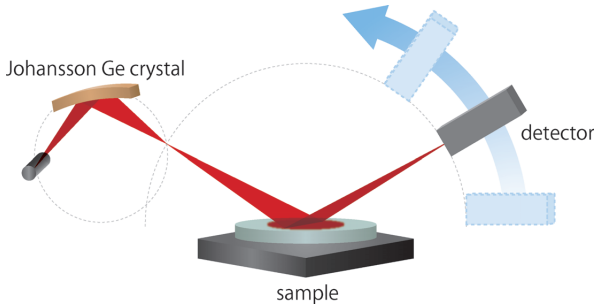

Fig. 8. Schematic diagram of Kα1 unit+Bragg-Brentano focusing method.

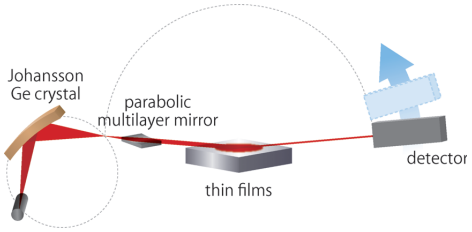

Fig. 9. Schematic diagram of Kα1 unit+parallel beam method.

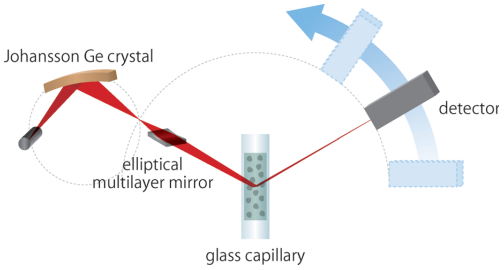

Fig. 10. Schematic diagram of Kα1 unit+convergent beam method.