Highly versatile multipurpose X-ray diffractometer

SmartLab 3

1. Introduction

SmartLab 3 offers continued refinement of the original ease of use features awarded the R&D 100 Award in 2006: automatic alignment, component recognition, cross beam optics and a five axis goniometer. Award winning guidance software recognizes installed components and seamlessly integrates them into data collection and data analysis methods. The Cross beam optics module offers permanently mounted, permanently aligned and user selectable optical geometries for various diffraction experiments. As an example, one can choose a Bragg–Brentano and parallel beam combination for measurements of both powders and thin films without the need for instrument reconfiguration. One could also choose a Bragg–Brentano and focusing transmission combination to measure organic materials in both transmission and reflection modes. The fifth axis or in-plane axis of the SmartLab allows the measurement of structures that are in the surface plane of the sample. This allows the measurement of extremely thin films and depth profiling in coatings. The SmartLab 3 system further extends application capability with the HyPix-400, a next generation 2-D detector. This hybrid pixel array detector offers the highest resolution and count rates available today. It is fully manufactured and integrated into the SmartLab 3 system by Rigaku and, as such, offers the superior ease of use pioneered by Rigaku in the original SmartLab system model. The SmartLab 3 configured with a HyPix-400 detector operates in 0-, 1-, and 2-D models without the need to exchange a detector.

2. Unique features

2.1. A true multipurpose X-ray diffractometer

Modern X-ray diffractometers are expected to support multiple applications; *e.g.*, powder diffraction, thin film analysis, small angle X-ray scattering, residual stress and texture, to name a few. However, with the increase in complexity and sophistication that accompanies a multipurpose instrument comes the risk of a decrease in usability. How do you know for certain that you or your fellow researcher is selecting the best optics for each application? When switching between complex configurations, how can you be absolutely certain that your instrument remains aligned and that the data that you measure is of the utmost quality? The SmartLab 3 answers these questions in two ways. First, the instrument recognizes the specific optic components that are currently mounted on the diffractometer and checks the configuration against the type of measurement that you have selected. If the current configuration is not the best one for your intended measurement, the software suggests how you should change the hardware configuration for the type of application selected. Second, after the proper hardware components have been added to the instrument, the instrument performs an automatic alignment—a unique feature of Rigaku and the only true way to know that your instrument is ready to collect the high quality data that your research demands.

2.2. HyPix-400: Next generation 2-D detector

In recent years, two-dimensional detectors have become popular for powder and thin film X-ray

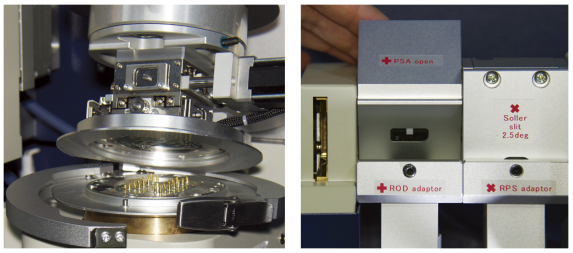

Fig. 1. Optics component recognition to identify the mounted optics. User Guidance software checks the optics and guide the operator to configure the best possible optic setup for application.

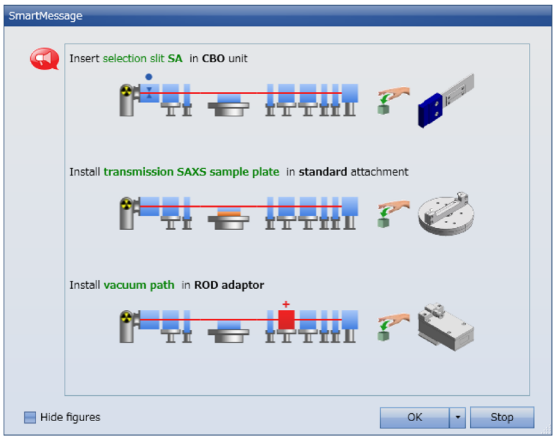

Fig. 2. The User Guidance software is suggesting to configure a selection slit at cross beam optics, transmission sample stage and vacuum beam path for transmission SAXS measurement selected by an operator.

diffraction. With the SmartLab 3, Rigaku introduces the HyPix-400, a semiconductor hybrid pixel array detector that was specifically designed for multipurpose X-ray diffractometers. Its large active area of 400 mm^2, high angular resolution of 100 μm square pixel size that is equivalent with 0.02° angular resolution and ultra-high dynamic range of greater than 10^{10} cps or 10^6 cps/pixel make it the perfect, affordable, 2-D detector solution for a large variety of applications, including powder and thin film diffraction.

2.3. 5-axis goniometer gives additional information on thin film samples

Thin film diffraction measurements have grown steadily over the last two decades. In some large shared X-ray facilities, thin film work now constitutes 50% of the work being done. Because of this, it is now very important to have a diffractometer that has the most flexibility in measuring the unique properties of thin film materials. Rigaku's unique solution to this problem is to include a fifth axis of rotation for the goniometer. This design enables the thin-film researcher to perform an "in-plane" scan, where the detector rotates in a plane parallel to the sample surface. This experimental configuration provides unique information for thin film materials; *e.g.*, in-plane lattice constants

Fig. 3. HyPix-400, a 2-dimensional detector based on semiconductor hybrid pixel array detector (HPAD) technology.

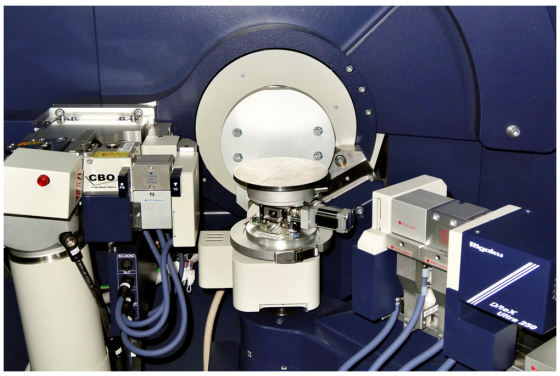

Fig. 4. Unique in-plane axis drives detector in a plane parallel to sample surface, which enables to see in-plane lattice parameters, crystal structure as a function of depth from the sample surface.

Table 1. List of applications which supports automated optics alignment.

Supported configuration for auto alignment	· Bragg–Brentano · Parallel beam · Parallel beam kα_1 · Focusing Debye-Scherrer configuration · Micro-area X-ray diffraction · Stress/texture · In-plane X-ray diffraction · SAXS/U-SAXS · Non-ambient chambers

and in-plane preferred orientation as a function of depth from the sample surface. If you are interested in thin film diffraction, this is a feature that will give you information that cannot be obtained on competitive diffractometers.

2.4. Maximize your uptime

Changing hardware configurations or consumables on some diffractometers is so daunting that people often invite their service engineer to perform the task. This can be costly and time consuming. Research stops when you are waiting for your service engineer to

realign or configure your instrument. Rigaku addressed this issue years ago by designing and incorporating an automatic alignment system into a diffractometer, and this useful and safety oriented design is included in the SmartLab 3. The optics configuration on the SmartLab 3 is self-aligned. From the tube height to the monochromator alignment, all of the optics alignment is done automatically under computer control. This feature drastically reduces down time and cost of ownership of the instrument, and it allows you to be confident that your instrument will always be in aligned condition.