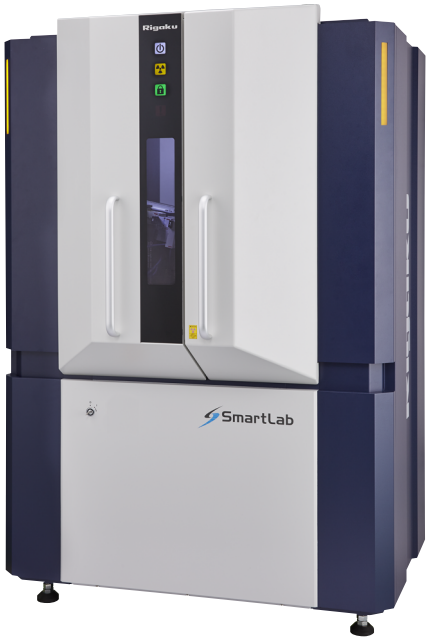
Automated multipurpose X-ray diffractometer

SmartLab SE



1. Introduction

SmartLab SE, which includes a semiconductor detector as a "standard" component, is Rigaku's newest automated multipurpose X-ray diffractometer system. Customers can select either the "2D" or the "1D" version of this system. If customers select the "2D" model, they can easily determine the degree of preferred orientation and coarse grain size effects from the shape of Debye-Scherrer rings using the hybrid pixel array detector "HyPix-400". The SmartLab SE configured with a HyPix-400 detector operates in 0, 1, and 2D models without the need to change the detector.

This system also offers the original ease-of-use features of the SmartLab system: automatic alignment, component recognition, and Cross Beam Optics. The guidance software recognizes installed components and seamlessly integrates them into data collection and data analysis methods. The Cross Beam Optics (CBO) module offers permanently mounted, automatically aligned and user-selectable optical geometries for various diffraction experiments. For example, one can choose a Bragg-Brentano optics and parallel beam optics combination for measurements of both powders and thin films without the need for instrument reconfiguration. One can also choose a Bragg-Brentano optics and focusing transmission optics combination to measure organic materials in both transmission and reflection modes.

2. Unique features

2.1. A truly multipurpose X-ray diffractometer with user guidance function

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. SmartLab SE has the measurement guidance software "SmartLab Studio II". This software suggests the optimal hardware configuration and settings for specific application measurements. The software will determine which optics are most appropriate for a given application, determine the instrument settings and execute the measurement, offering a completely automated measurement sequence.

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, it performs an automatic alignment—a feature unique to Rigaku instruments and the only true way to know that your diffractometer is ready to collect the high-quality

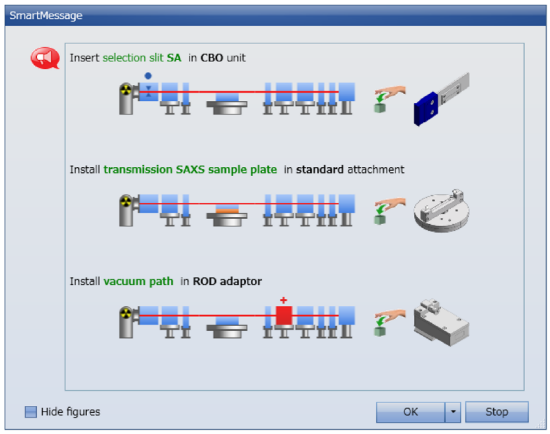


Fig. 1. The user guidance software SmartLab Studio II suggests the appropriate selection of a slit for the Cross Beam Optics, the sample stage, etc.

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

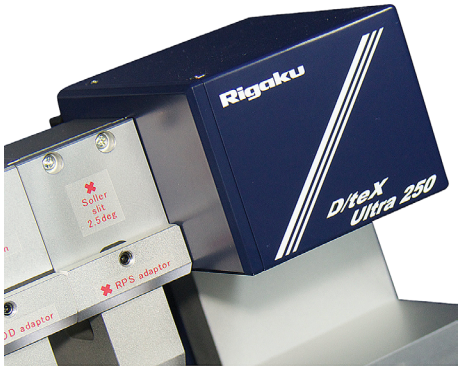


Fig. 3. D/teX Ultra250, a 1D silicon strip detector.

data that your research demands.

2.2. State-of-the-art detectors for high-speed measurements

SmartLab SE offers two types of semiconductor detector. One is a hybrid pixel array multi-dimensional detector, the "HyPix-400" (0D/1D/2D). Its large active area of 400 mm^2, high angular resolution with a 100 μm square pixel size that is equivalent to 0.02° angular resolution, and ultra-high dynamic range of greater than

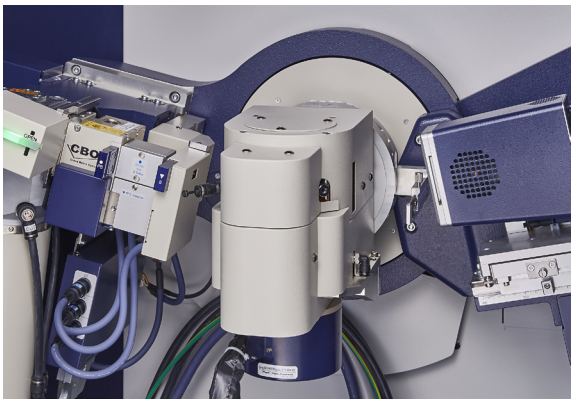


Fig. 4. DSC attachment.

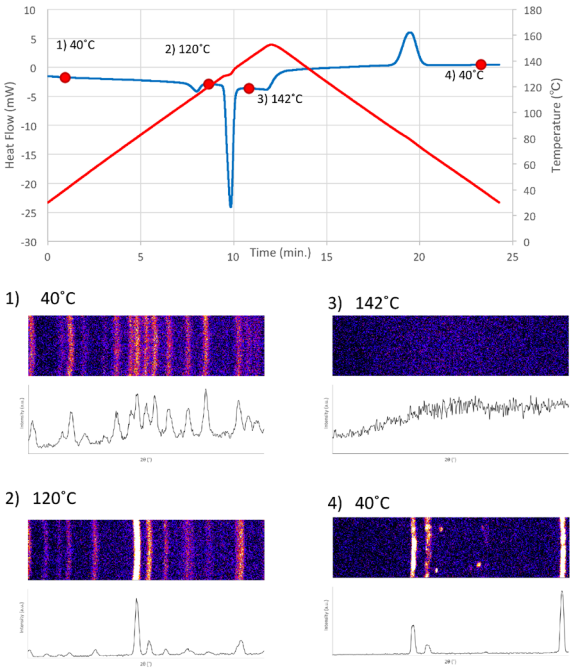


Fig. 5. Phase transition/melting behavior of tolbutamide, a therapeutic agent for diabetes, with the change of temperature.

10^{10} cps or 10^6 cps/pixel make it the perfect, affordable, 2D detector solution for a wide variety of applications, including powder and thin film diffraction. The HyPix-400 detector functions not only as a 2D detector but also as a 1D detector to detect even trace components due to an effect of the integrated intensity, and also functions as a 0D detector like a scintillation counter by simply switching modes in software.

Alternately, users can select a high-resolution, ultrafast 1D X-ray detector, the "D/teX Ultra250" (0D/1D). The D/teX Ultra250 detector supports high-speed Bragg-Brentano focusing measurements and is capable of acquiring wide-angle powder diffraction profiles in just a few minutes. Its high energy resolution, the distinguishing feature of semiconductor detectors, helps reduce the background during measurement.

2.3. Various attachments for *in situ* measurement

In situ measurement enables observing changes in sample state with variations in temperature and humidity at the same time. SmartLab SE supports a variety of *in situ* measurement attachments, such as for observing changes in the sample state with changes in humidity or temperature, and for observing changes in the sample state before and after a thermal reaction when combined with the DSC attachment. With the combination of an *in situ* attachment and a HyPix-400 detector, real-time measurements are achievable, allowing the identification of brief structural changes, as well as large grains and orientation.