Integrated X-ray diffraction software
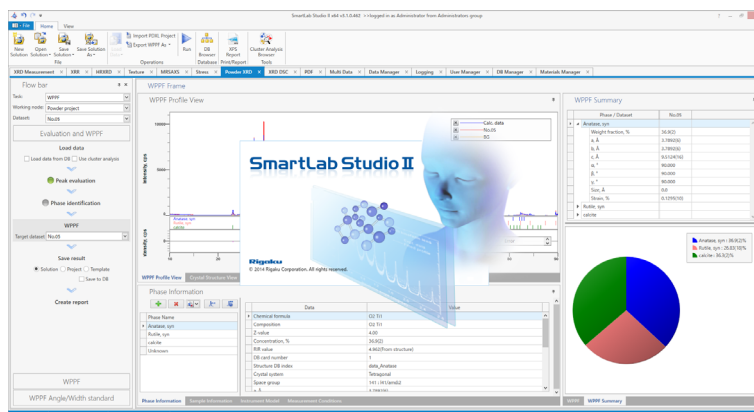
SmartLab Studio II
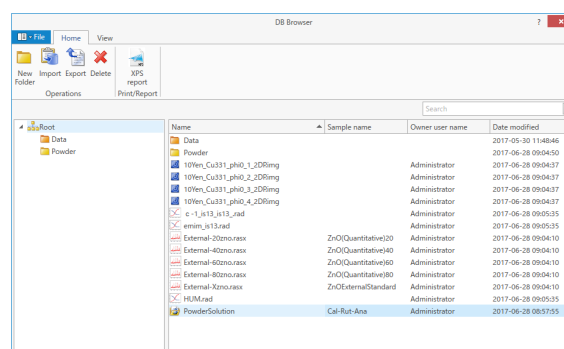
─New features─

1. Introduction

SmartLab Studio II is an integrated X-ray diffraction software package for making both measurements and analyses using SmartLab, an automated multipurpose X-ray diffractometer. Two years ago[1], the user guidance feature, flow bars, chart control, report manager, SQL database[*1], and plugin modules were introduced. Now we would like to announce several new features of SmartLab Studio II for the SmartLab SE system which was launched to the market in April, 2017.

2. Enhancement of ER/ES features

SmartLab Studio II fully complies with the regulations and guidelines for pharmaceutical production and sales (21 CFR Part11, EU-GMP Annex11, PIC/S). The User Manager, Audit Trail Viewer[*2], and SQL database support all the required features, such as access restriction and management to the system by a user ID and password, setting permissions to each user account, guarantee of data integrity, electronic signature, audit trails of operator entries and actions, and so forth. Archiving electronic records and a backup function are available so you can preserve the large number of data sets that have been collected and analyzed over a long period, even in one PC.

3. New database browser

A new database browser (Fig. 1) provides almost the same features as those of Windows Explorer: copy data, create a folder, move data to a folder, rename data, etc. Compared to the legacy list-view-type browser, it is much easier to handle data sets in the SQL database as if they were stored in the Windows file system. It is, for example, possible to restrict browsing data sets from any other users except the data owner (creator) using data sharing settings. When you use SmartLab Studio II in ER/ES mode[*3], only authorized users can delete or overwrite data. Edited data will be saved with the same name and a new revision number.

4. Transfer data to analysis plugins

When you wanted to perform data collections and analyses using the previous version of SmartLab Studio II, you had to take the following steps: (1) Collect data with the XRD Measurement plugin. (2) Save the collected data. (3) Switch to the analysis plugin. (4) Load the saved data. With the new version, after data collection you only have to select the analysis plugin for your purpose from the Transfer Data menu. The data displayed in the XRD Measurement plugin will be loaded and displayed by the selected analysis plugin.

Fig. 1. A new database browser.

Since the data displayed on the main window is the target to be loaded, this new feature will reduce user errors caused by loading the wrong data. It goes without saying that the procedure of loading data is simplified.

5.   New features of the Powder XRD plugin
5.1.   Navigation flow bars prepared for each application

PDXL Integrated X-ray Powder Diffraction Software arranges the buttons for every application and function—Load Data, Save Project, Data Process, Create Report, etc.—in a single flow bar. That's why the PDXL user had to select the required applications and functions during his/her analysis. By contrast, the Powder XRD plugin, a new model for powder diffraction analysis, prepares several individualized navigation flow bars that contain the functions required for each application, such as phase identification, quantitative analysis, %crystallinity analysis, Rietveld analysis. Follow the flow bar, and you will be able to load the data, do the analysis, save the results, and create a report. The flow bars were designed to allow the user to switch from one application to another, which will satisfy skilled users in the powder diffraction analysis field.

5.2.   XY mapping display

An XY mapping display feature is now available in the Powder XRD plugin. Peak search results or other analysis results can be shown on an XY map. After loading a set of XY mapping measurement data and analyzing all the data, the analysis results can be displayed as shown in Fig. 3. In addition to XY mapping measurement data, various types of map data can also be created by assigning any physical values (temperature, axis positions, etc.) to the X and Y axes.

6.   Analysis of TDI scan[*4] data using a 2D detector

When you perform a TDI scan using a Rigaku HyPix series 2D detector, 2D data will automatically be converted and saved as 1D profile data in the 2θ-I format. No dedicated 2D data processing software is necessary. Moreover, by making use of the data-transfer feature described in Section 3, measured data can be loaded by an analysis plugin as soon as 2D data measurement is complete.

7.   Clustering (Cluster analysis)

The cluster analysis module is independent of the other analysis plugins in SmartLab Studio II (Fig. 4). Cluster analysis can be performed when multiple data sets of reflectivity, rocking-curve, powder diffraction data, or even 2D are loaded with the cluster analysis module. After clustering, you can proceed to an analysis plugin by loading the data sets included in the selected "cluster". If you set a reference data set in advance, the cluster analysis module will retrieve and extract data similar to the preset reference data from the SQL database and/or the file system. This may be a convenient function when you want to extract target data sets from data sets stored in the past.

Thus, using the new SmartLab Studio II software,

Fig. 3.   XY mapping data display.

Fig. 2.   A navigation flow bar.

Fig. 4.   Cluster analysis module.

data handling and management become much easier, not to mention measurements and analyses. In particular, several features have been enhanced for handling a lot of data sets, which will contribute to reducing the time of analysis and report creation.

*1 SQL database

To consolidate all the information such as user accounts, collected data, analysis results, etc. SmartLab Studio II utilizes the Microsoft SQL server database. Data security is tightened compared to the file system, and it is easier to manage loading or deleting data in the database.

*2 Audit Trail Viewer

A plugin displays audit trails in ER/ES mode. This plugin provides a good filtering function to filter the audit trails under several conditions. You can easily display only the desired part of the audit trails.

*3 ER/ES mode (Electronic Record and Electronic Signature)

Use the ER/ES mode under conditions requiring the integrity of electronic records and the need to add electronic signatures. It is possible to electronically sign analysis results in this mode. When creating a report from signed analysis data, signature information is shown on the report. The history of user entries and operations is recorded in the database as an audit trail.

*4 TDI scan

A high-speed scan method using 1D strip detectors or 2D pixel detectors. Since the intensities collected by a large number of strips or pixels can be accumulated due to the high position sensitivity of the detectors, high intensity will be obtained even with a high-speed scan.

Reference

(1) *Rigaku Journal (English version)*, **31** (2015), No. 2, 25−26.