Integrated X-ray diffraction software
SmartLab Studio II
—One-stop X-ray diffraction software for both measurement and analysis—

1. Introduction

SmartLab Studio II is an integrated X-ray diffraction software package for SmartLab 3, an automated multi-purpose X-ray diffractometer. The package covers the full spectrum of operations required for X-ray diffraction analysis, including measurement, analysis, data display and reporting on a single platform. SmartLab Studio II is designed from the ground up with ease-of-use in mind, so that even novice users are able to quickly master their X-ray diffraction systems. This article introduces some of these features.

2. User guidance

To make an X-ray diffraction measurement correctly, it is necessary to install appropriate optical devices for the application and to set proper measurement conditions. Optics alignment and/or sample alignment are sometimes required. However, without ample experience making measurements it can be difficult to select optical devices and set alignment/measurement conditions. The User Guidance feature in SmartLab Studio II helps to make all of this easier, even for those without much experience. All that you have to do is to click the OK button after installing optical devices according to the instruction message displayed. Then, you will obtain data equivalent to that of an expert. If you install the wrong optical device(s), the automatic optics recognition feature will instruct you to replace them with the correct ones.

3. Flow bar navigation

The procedures of both measurement and analysis are navigated via the flow bar. A measurement usually consists of the following four steps:

(1) optics setup and alignment
(2) mounting sample(s)
(3) sample alignment
(4) data measurement.

These steps are displayed on the flow bar. You only have to enter just a few pieces of information such as the name of the data to save. Then, the measurement will start and data will be collected. A flow bar based on your application will guide you through each step of data analysis (Fig. 2). Using this interface, you can perform the analysis step by step, from loading your data through report creation. Each button has a one or two-line

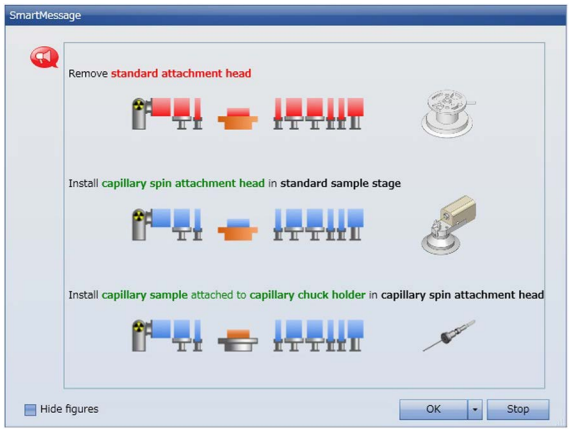

Fig. 1. Instruction message to change optical devices.

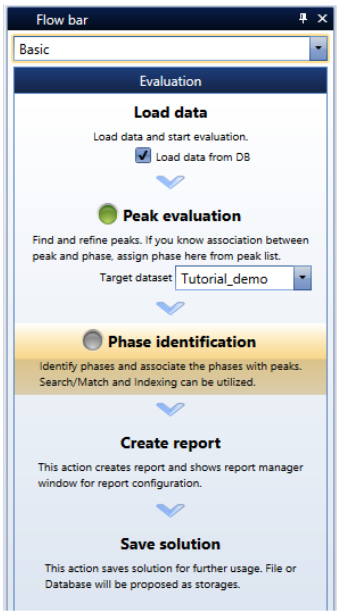

Fig. 2. Flow bar of Powder XRD plugin.

description so you can proceed with your analysis with a good understanding of the processing content of each step.

4. Chart control with rich features

Chart control is incorporated to display a variety of graphics such as topo-map and other 3D visualizations, as well as 1D profile data and 2D image data. Fast, beautiful graphics make your data come to life using DirectX (Fig. 3). Since all the applications use the same interface, navigating your data with zoom, rotation, color assignment and other attributes is easy to learn.

5. Report Manager

The Report Manager enables you to customize the content and layout of a report with just the mouse. You can modify what and where to print and display information in the report preview window. Each item can easily be shown/hidden. The created report can be printed and saved as a file in a variety of formats such as PDF, RTF, XLSX, JPG, and so on.

6. Consolidate information

Materials information, which used to be prepared for each application, is now well-organized in one materials database and it can be managed in an SQL database. User information, logging information, collected data, analysis results, and macros are also managed in the same SQL database. Even when multiple users use SmartLab Studio II, you can manage all information centrally. You can filter information keyed to your user name, you can share information with all users, etc. If a network license is available, the users in the same local area network can share a single SQL database, which is very convenient if your SmartLab 3 has been installed as a shared system. Since the SQL database makes data management (in terms of security) very easy, SmartLab Studio II can be configured to be compliant with key regulatory standards, such as FDA21 CFR Part11.

7. Applications & features divided

The features of SmartLab Studio II are divided into several "plugin modules" organized by purpose. You only need to load the plugins you will use. There is one measurement plugin and seven analysis plugins as shown in Table 1. There are also several common plugins included in SmartLab Studio II. For example, in the Automation plugin, which is one of these plugins, you can arrange functions of measurement and analysis to create an "analysis macro". After you set conditions for the arranged functions in advance, you can always perform automated measurement and analysis under these conditions, greatly improving the efficiency of your work. This feature is incredibly convenient for process control or quality control departments.

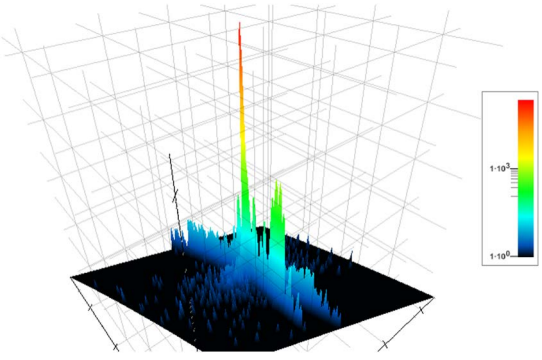

Fig. 3. 3D display of Chart Control.

Table 1. List of measurement and analysis plugins.

Plugin	Description
XRD Measurement	Make measurements using SmartLab 3
Data Manager	Display/process/calculate 1D/2D data.
Powder XRD	Perform qualitative, quantitative, Rietveld analysis.
XRR	Evaluate thickness, density, roughness based on X-ray reflectivity of thin-film samples.
HRHRD	Evaluate thickness, composition, relaxation degree based on rocking curve and reciprocal space map of epitaxial thin-film samples.
Texture	Evaluate orientation degree and crystal orientation based on pole figures and ODF analysis.
MRSAXS	Evaluate shapes and size distributions of nanoparticles from SAXS data.
Stress	Evaluate residual stress of samples from 1D/2D data set.