Technical development at the Materials Research end-station

W. Oehme[1], S. Dienel[1], U. Strauch[2], F. Eichhorn[3], N. Schell[3]
[1] Department of Research Technology
[2] Project Group Rossendorf Beamline at ESRF
[3] Institute of Ion Beam Physics and Materials Research
Forschungszentrum Rossendorf, P.O. Box 510119, 01314 Dresden, Germany

Introduction

This report summarizes the most important technical development realized during the last two years in the field of experimental automation at the materials research end-station of ROBL. It has been carried out by members of the Department for Research Technology at the FZR in collaboration with the scientists in Grenoble and comprises special tasks in the fields of mechanical construction, electronic instrumentation and engineering, and particularly, software development. The main goals of these developments were:

- to increase the reliability of the components
- to integrate new equipment into the common experimental concept
- to contribute to a high degree of automation for unattended beamline mode
- to improve the visualization of results in real time.

General infrastructure

The previously used two independent workstations for optics and experimental control in the control cabin E2C were replaced by 2 SunRay-1 terminals each equipped with 18-inch LCD monitors connected to a new centralized workgroup server for the whole beamline (Sun-E250). This increased the reliability of the total system and reduced both noise and necessary space inside the cabin.

Software development

Using the PSD (linear position sensitive detector) a large amount of data is generated (up to 500 * 8k - 32 Bit per scan). This data is stored in a *spec*-typical format [1] which in this form is not easy to analyze *after* and practically impossible to evaluate *during* the experiment. This, however, is important in order to correct any spurious effects for optimization of the experiments in real time. For this reason the following three programs were developed in collaboration with scientists of the Institute of Ion Beam Physics and Materials Research:

1. *mcaView* [2]**:** This program is based on a professional XRT/3d-Widget [3] and presents the measured data in a hardware-like manner. The angles of the scan and the channel numbers of the MCA (multi channel analyzer) are taken as the *X*- and *Y*-axes. The counts of the MCA channels are drawn in *Z* direction. The data can be presented in different modes according to the predefined facilities of the XRT/3d-Widget. The most preferable mode is the *contour plot* in a 2D manner with the *Z* values presented in a color scale (see Fig. 1). Since presenting the data in a 3D manner can be very time-consuming, an automatic binning is performed depending on the amount of data to be presented. The program can be used in a *quasi-online* mode and also *offline* (for later data analysis and representation). *Quasi-online* means: The measurement performed by the program spec and *mcaView* are two completely different processes. They only share the same data file. At every time the length of this data file changes, *mcaView* would perform a new presentation.
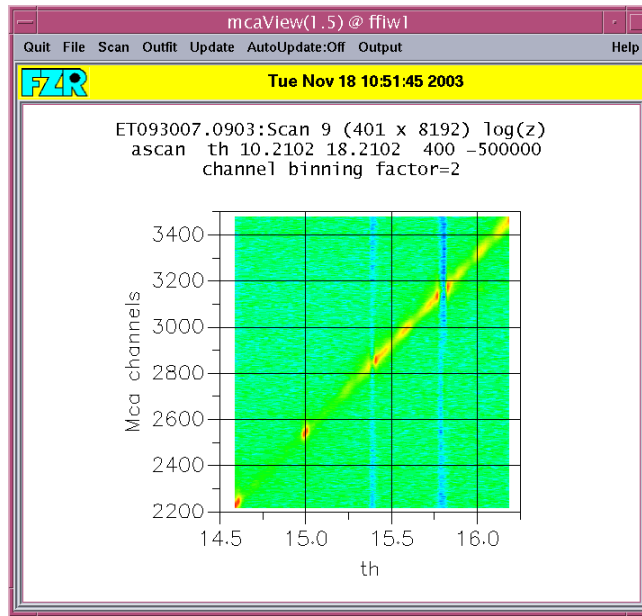
Fig. 1: Example of mcaView's output in contour mode.

2. ***psdView*** [4]: Based on the application *mcaView*, a second application was developed that performs a reciprocal space mapping (RSM). In this way the data can be presented angle-independent often better comparable to literature representations. The data had to be represented as pixel graphics in reciprocal space co-ordinates calculated from the diffractometer scattering angle and predefined calibration parameters of the PSD via

$$tth_{PSD} = tth_{GON} + (PSD_{channel} - PSD_{centre}) / PSD_{slope} \quad \text{and}$$

$$Q_x = 2\pi / \lambda * (\cos th_{GON} - \cos (tth_{PSD} - th_{GON})) \quad [1/nm]$$
$$Q_z = 2\pi / \lambda * (\sin th_{GON} + \sin (tth_{PSD} - th_{GON})) \quad [1/nm]$$

with the zero point PSD_{centre}, the resolution PSD_{slope}, and the wavelength λ taken from a *selection dialogue box*. Each measured value belonging to such a Q_x-Q_z-tuple is transformed into a scale of 100 colors either in a *linear* or in a *logarithmic* manner. Depending on the size of the window on the screen and the chosen clipping, the Q_x and Q_z co-ordinates have to be mapped into pixel positions (since this mapping can lead to some measured values being shown at the same pixel, always the color belonging to the highest measured value is set). The program can be used in a *quasi-online mode*.

An example is shown in Fig. 2. The data come from measurements of a semiconductor superlattice of 100 double layers, each of which consists of 5 nm GaAs and 7 nm $Al_{0.3}Ga_{0.7}As$, deposited by MOCVD (Metal Organic Chemical Vapor Deposition) on GaAs and measured in the neighbourhood of the GaAs(002) reflection. The nearly equidistant points (stripes, respectively) are the SL peaks of increasing interference order (counted from the centre).

3. ***psdConv*** is a Windows program which converts measured data stored in the *spec* dedicated format into text files by performing the same RSM as for *psdView*. It produces 3D-tuples in reciprocal space which can be used as input for a professional 3D program). Additionally, the generated data can be reduced by selecting a low limit value below which the data are not converted.
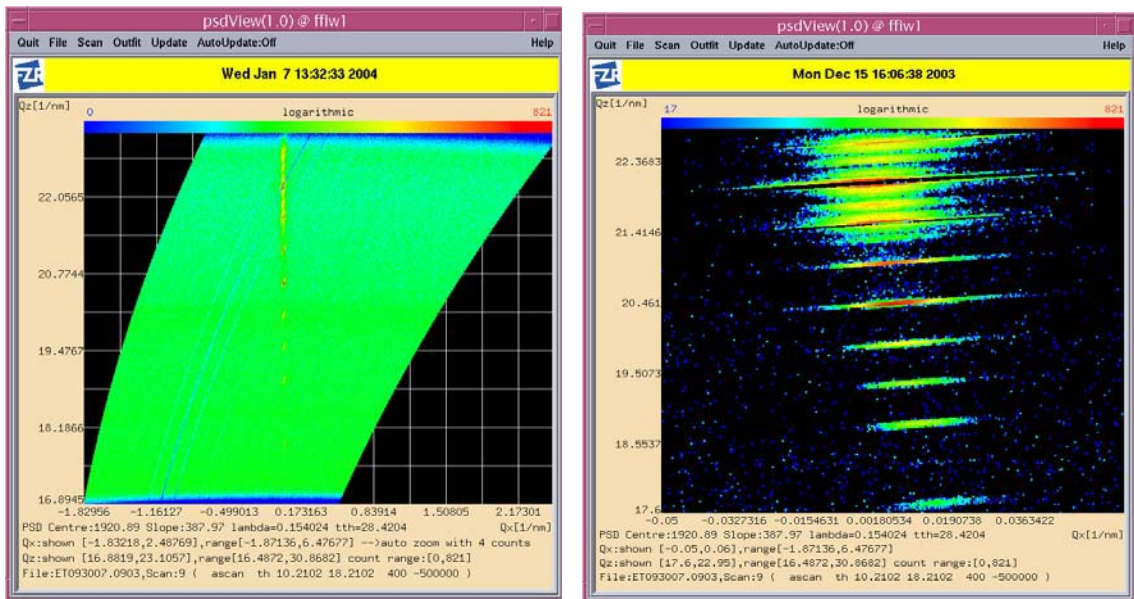
Fig. 2: Run visualization (left) of a rocking curve with the PSD of a GaAs/AlGaAs ML in the neighbourhood of the GaAs(002) reflection. The red and yellow points are SL peaks, the blue stripes are low-intensity artifacts. The zoomed presentation (right) uses 'large' pixels.

Electronic stepper motor controller switch

An example of electronic engineering is shown in Fig. 3. The 6-circle HUBER-diffracto-meter is controlled via dedicated electronics in *spec*[TM]. But with the 2-dim. CCD detector SMART with its electronics from Bruker, the two systems use different types of stepper motor controllers. As some experiments are easier performed when directly programming the movement of the diffractometer via the SMART software, we have realized an alternative access to four of the axes of the diffractometer (required for the SMART system). We developed a special module drive in a control unit which can be switched between the two types of stepper motor controllers. The four modules offer switchable inputs which provide electronically compatibility to either SMART CONTROL or the VPAP-module in the VME-system and serve the drives of the diffractometer axes at their output. The main difficulty in was to keep the original compatibility to separate communication.

Fig. 3: Axes Switch Unit (left) and one of the controllers (right) developed in the Department of Research Technology of FZR.

References

[1] Certified Scientific Software, *spec*[TM] *X-Ray Diffraction Software*, User's Manual (2001)
[2] W. Oehme, *mcaView*, Internal Report ROBL (2003)
[3] KL Group Inc., *XRT/3d*[TM] *for Motif*, Programmer's Guide & Reference Manual, V2.1 (1994)
[4] W. Oehme, *psdView*, Internal Report ROBL (2003)