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LabVIEW interface with Tango control system for a multi-technique X-ray spectrometry IAEA beamline end-station at Elettra Sincrotrone Trieste

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ABSTRACT

A new synchrotron beamline end-station for multipurpose X-ray spectrometry applications has been recently commissioned and it is currently accessible by end-users at the XRF beamline of Elettra Sincrotrone Trieste. The end-station consists of an ultra-high vacuum chamber that includes as main instrument a seven-axis motorized manipulator for sample and detectors positioning, different kinds of X-ray detectors and optical cameras. The beamline end-station allows performing measurements in different X-ray spectrometry techniques such as Microscopic X-Ray Fluorescence analysis (μXRF), Total Reflection X-Ray Fluorescence analysis (TXRF), Grazing Incidence/Exit X-Ray Fluorescence analysis (GI-XRF/GE-XRF), X-Ray Reflectometry (XRR), and X-Ray Absorption Spectroscopy (XAS). A LabVIEW Graphical User Interface (GUI) bound with Tango control system consisted of many custom made software modules is utilized as a user-friendly tool for control of the entire end-station hardware components. The present work describes this advanced Tango and LabVIEW software platform that utilizes in an optimal synergistic manner the merits and functionality of these well-established programming and equipment control tools.

1. Introduction

LabVIEW is a graphical dataflow programming language developed by the National Instruments Corporation which is widely used for development of data acquisition, automation and control software. LabVIEW intuitive coding enables the creation of advanced control applications in a relatively short time. The graphical user interface (front panel) of Virtual Instrument (VI) can be also created easily offering wide flexibility for further modifications and development. LabVIEW supports vast variety of hardware devices produced by a different suppliers by the use of dedicated VI's or other specific tools such as Dynamic Data Exchange (DDE) or Dynamic Link Library (DLL). A wide variety of applications [1–4] have shown the advanced possibilities that LabVIEW provides for scientific instrumentation controlling.

Tango is a powerful object oriented control system toolkit designed for control of various devices. It is an open source software which was developed through the collaboration of four synchrotron radiation facilities namely ALBA, ELETTRA, ESRF and SOLEIL [5,6]. The main feature of Tango is to provide a communication bus between different hardware modules (supporting C++ and Java programing languages) and GUI tools. The GUI can be created in one of the supported languages namely Matlab, LabVIEW or Igor. Up till now several examples of use of the Tango framework bound with the LabVIEW based GUI have been presented [7–9].

In this work we present a GUI created with LabVIEW which is bound to a Tango device servers to control the hardware components of a multipurpose X-Ray spectrometry facility that operates as end-station of the newly developed XRF beamline at Elettra Sincrotrone Trieste [10]. Using the modular features of LabVIEW code and Tango framework, the main aim of this approach was to create a functional, user friendly and easy-to-expand interface that will be in support of the broad functionality of the beamline. Some examples of application of the end-station are also shown in

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present paper to demonstrate the modalities and the reliability of the control system.

2. Instrumentation

The X-ray spectrometry beamline end-station was designed to enable an optimum and functional integration of different X-ray spectrometry based analytical methodologies in one single facility. The prototype facility is described by Lubeck et al. [11] and a brief overview of similar follow-up developments is given in [12]. The end-station consists of an ultra-high vacuum chamber (UHVC) which houses a motorized seven-axis manipulator (Huber, Germany) and different types of X-ray detectors and digital cameras. A load-lock chamber is attached to the main UHVC allowing, with the help of a manual transfer system, the fast exchange of samples for measurement. The entire system is mounted on a three-axis motorized stage that comprises two linear and one rotational axes (Astrofein, Germany) to support the alignment of the whole end-station versus the incident beam of synchrotron radiation. The motorized seven-axis manipulator is composed of four linear stages ('X', 'Y', 'Z') and three rotational axes ('Theta', '2Theta', 'Phi') used to provide proper orientation of both the analyzed sample and X-ray detectors as required by the experiment to be conducted. In particular, the sample manipulator allows three translations in Cartesian geometry and rotation around two axes. An additional rotational axis and linear stage are used for the movement of X-ray detection systems with respect to the direction of the synchrotron beam or/and sample surface orientation.

An ultra-thin window Silicon Drift Detector (SDD) (Bruker, Germany) mounted in fixed position (90° in respect to the primary beam) is used for the detection of secondary X-rays from the sample. A picoammeter (Keithley, USA) measures the photo-current induced by the direct beam or the beam reflected from the sample surface in one from a set of five selectable photodiodes (Hamamatsu, Japan and Optodiode, USA). The flux of the primary X-ray beam is monitored with use of diamond membrane detector (Dectris, Switzerland). The temperature of all stepper motors is monitored with thermocouples connected to an input module (Advantech, USA). Two optical color cameras mounted outside the UHVC are used for the inspection of the sample environment. The wide-view camera (Lumenera, Canada) integrates a telecentric lens, whereas the narrow-view camera (PCO, Germany) is coupled to a long distance microscope (Infinity, USA).

All hardware components of the beamline end-station are connected to a Server PC placed inside the experimental hutch of the beamline. The Server PC is connected inside the beamline control room with the Client PC which runs the GUI program via a Gigabit Ethernet Switch. The manipulator controller, picoammeter and thermocouple input module as TCP/IP devices are connected to the server PC via Gigabit Ethernet Switch as well. The SDD is connected directly to the Server PC via USB port. Both cameras are connected directly with the Client PC via USB port with the use of a USB extender. The Server PC is also connected to the Elettra Beamline Control System via separate Ethernet Switch to read the parameters of the monochromator and the beamline. A clone of the server PC is used as a backup in the case of a disaster failure of the server. The clone is running database and Tango servers for all devices and can replace the server PC in any time by connecting it into the network. The schematic diagram of the connections between devices is shown in Fig. 1.

3. Control software

3.1. Tango control system

The control of all UHVC hardware components, except optical cameras, is achieved by separate software modules – Tango Device Servers (TDS, as defined by Tango terminology), which makes the system easy to expand. All developed TDS are written without any GUI and cannot be accessed by beamline end-users. Also they are self-sufficient for running measurements. These features simplify programming and increase robustness of the system. The modules are organized in two-level hierarchy. The low level TDS are independent of each other and they communicate with a corresponding hardware component on one side and one common high level module on the other side. The high level module is used to acquire data from all the instrumentation components. There is also one dedicated module called replicator which can communicate with Elettra Beamline Control System.

The high level module, called UHVC TDS, is capable to run in two distinguished modes: "scan mode" which acquires data synchronously with both sample and detector movements, including a single position scan, and "no-scan mode" which acquires data asynchronously without any sample or/and detector movement. The "no-scan mode" is mainly used for measurements at fixed

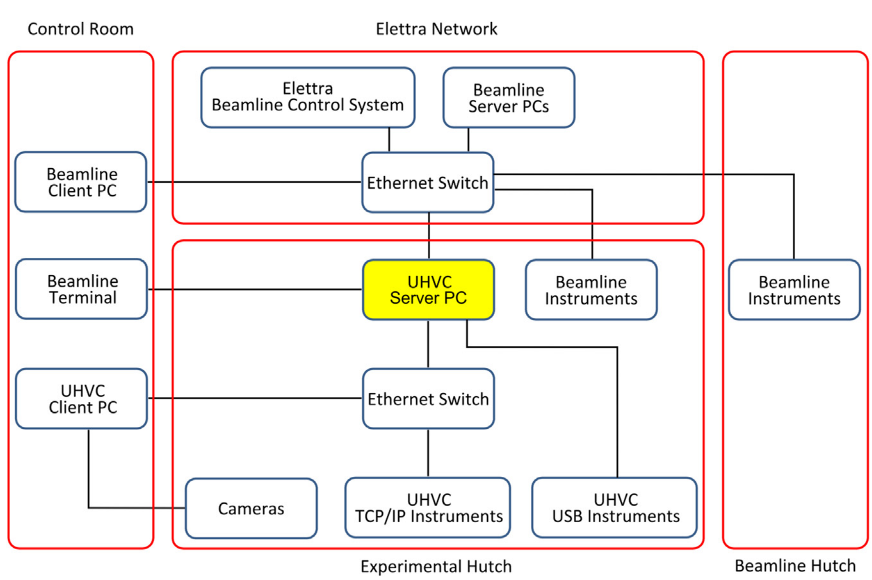

Fig. 1. The schematic diagram of the UHVC instrumentation.

geometry as well as for setting and fine tuning each of the mentioned instruments by monitoring parameters instantaneously. In the “scan mode” the module can perform measurements following the protocol of the chosen combination of supported analytical techniques.

In a typical “scan mode” experiment, the acquisition is implemented inside a thread which waits for multiple events to be signaled or set. The events are queued and handled according to their level of priority. The events can be internal – signaled by the thread or external – signaled by the user from a GUI program (i.e. start, stop acquisition), low level modules (TDS) or a software timer. During scanning procedure the internal events: (1) move sample/detector to a new position, (2) collect data from low level modules until the preset time is reached, (3) store collected data, are set and reset in such order that the following procedure is repeated until all points are scanned. In any of the previous procedures, also called states, an external event can be signaled. In stage (2), the thread can receive an event or pool TDS. For the purpose of pooling, the timer event is generated by the software.

The raw data collected at every new position are stored on the disk using HDF5 (under current development) or simple ASCII formats. The type of real time measurement, performed in stage (2) is defined by the user from the GUI program prior to start of the measurement.

3.2. Graphical user interface code design

The fundamental LabVIEW architecture of state machine was chosen to create the block diagram of the GUI Virtual Instrument (VI) as defined by LabVIEW terminology. The schematic diagram of the state machine together with all possible transitions between main states is shown in Fig. 2. During the measurements the states are continuously switched between “CheckStatus” and “UpdateScan” or “UpdateAcquisition”. Otherwise, when the GUI is idle it is kept in the “CheckStatus” state. The typical main loop speed is 10 iterations/s and at each iteration a different state is executed. The “Initialisation” state checks the status of Tango server and which devices are in use. It is also responsible for setting the appearance of all indicators and displays to harmonize the GUI appearance and settings stored by Tango server. The “UpdateScan” state is responsible for collecting from Tango server and displaying the most recent matrix of measurement data gathered during the scan process. The “UpdateAcquisition” state is responsible for collecting data from the Tango server and displaying the most recent measured spectra. Finally, the “InitScan” state sends all scan settings (scanning area borders as well as map definitions) to the Tango server and initiates the measurement, whereas the “InitAcquisition” state initiates a single acquisition with a chosen

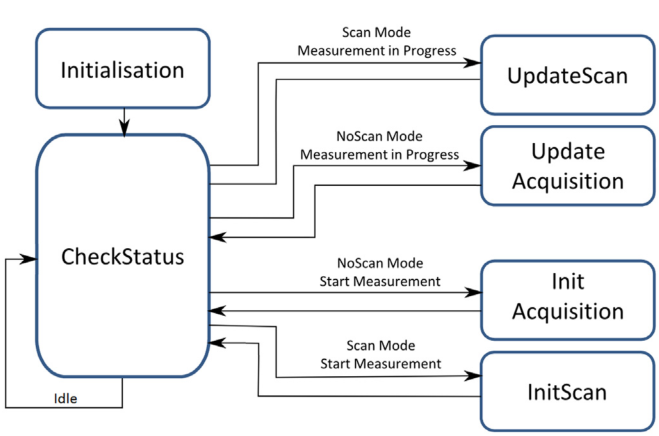

Fig. 2. Schematic diagram of state machine of GUI Virtual Instrument.

X-ray detector. The “CheckStatus” state incorporates an event structure which handles possible events caused by user interaction. The timeout event (done when no user interaction is detected) checks the actual status of the devices. The events handled by the “CheckStatus” state are connected with two types of user interaction. The communication events are responsible for data exchange with the Tango server i.e. starting/aborting measurements, sending presets, refreshing the displays, manual control of the seven-axis manipulator or the calibration of detectors. Other events are responsible for controlling the appearance of different parts of the GUI, mainly graphs and plots (showing/hiding cursors, adjusting scales etc.), as well as opening of external modules such as spectra/map windows or camera software. There are two separate sub-programs to operate both optical cameras. The communication between these programs and cameras is done by the use of dedicated subVI's provided by the respective manufacturers.

3.3. Interface functionality

The GUI functionality follows the UVHC TDS modes of operation. The appearance of the GUI front panel depends on the selected mode. There are two main parts of the GUI front panel: status window, which is common for both operation modes and I/O windows which are composed of two tab structures. Different devices and displays have its own dedicated tab that can be visible or not depending on the selected mode, whereas some of the tabs i.e. manipulator control and pressure preview remains visible in both modes of operation. The status window gives overall information about the operational status of the end-station instrumentation and Beamline Control System, as well as processes in progress. It also allows reading and controlling the setting of the incident beam energy. The main functions of the “no-scan mode” are the single acquisition of an X-ray spectrum using the SDDs, the access to the specific settings of all devices and the optimization of measurement conditions. It also gives the possibility to perform energy calibration of the SDDs spectra and to select spectral regions of interest (ROIs). The appearance of the GUI front panel in the “no-scan mode” is shown in Fig. 3.

In the “scan mode” it is possible to set and start a multidimensional scan that follows chosen measurement methodologies. This can be done by exchanging with UHVC TDS two types of variables. The first type is a scan coordinate matrix associated with movement of the manipulator stages or changing of the incident beam energy. The second type is a measurable quantity like a number of counts in a Region Of Interest (ROI) in X-ray spectra or a photodiode current. On this way the user can define any one- two- or three-dimensional distribution of a measurable quantity versus the scan coordinate(s). The distribution matrix is built by the UHVC TDS in real-time and can displayed real-time by the GUI. The GUI allows also the user to perform several multidimensional scans in pre-defined order with use of “Batch mode” operation. It is also possible to open an external window for data display and for performing simple mathematical operations on the acquired one-dimensional raw data such as differentiation of the plot and fitting with Gaussian profile. The external window gives also a possibility to point the target position for a given axis with the use of the cursor.

4. Examples of analytical applications

The main analytical methodologies supported by the developed control and data acquisition software are different variants of X-ray fluorescence (XRF) technique, X-Ray Reflectometry (XRR) and the application of X-ray Absorption Near Edge Structure Spectroscopy (XANES). XRF is a well-established and versatile

Fig. 3. The GUI in “no-scan mode”. Upper I/O tab shows SDD detector control panel and the lower I/O tab shows manipulator control menu together with Theta/2Theta visualization tool.

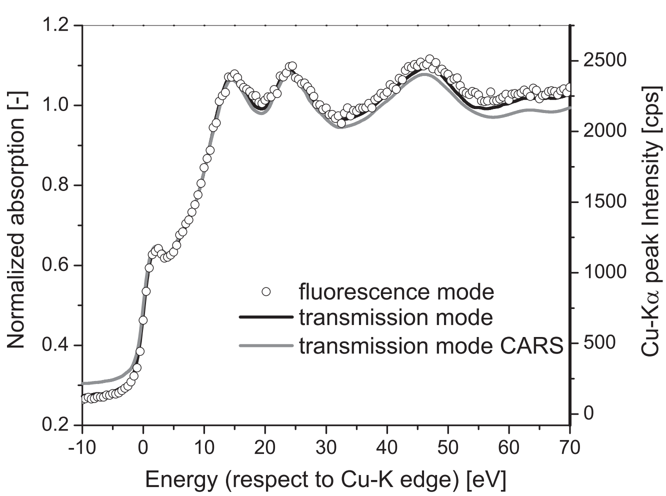

Fig. 4. XANES spectra of a 7-μm thick Cu foil measured via energy scan across the Cu-K edge in fluorescence and transmission modes.

analytical technique for studying the elemental content of different kinds of materials with sensitivity down to the ng/g concentration level for the best excitation/detection conditions, whereas XANES offers distinction of chemical forms of selected detected elements. Furthermore, the advanced sample manipulator installed at the end-station allows performing spatially resolved (micro-XRF, micro-XANES), surface (TXRF) and near surface angular dependent (GIXRF) measurements. In addition, the 2-theta goniometer coupled with the photodiode axis offers density/structural characterization of thin transparent samples/nanolayers by recording the intensity of the transmitted/reflected X-ray beam. The combined and synergistic use of these analytical methodologies is powerful and results in advanced characterization of complex samples. Some typical examples are reported here.

The simultaneous registration of signals of both SDD and photodiodes in energy-scan measurements enables the acquisition of XANES spectra in the so-called transmission and fluorescence mode. In Fig. 4, respective XANES spectra of a 7 μm Cu-foil (0.5 eV step, 1 s/step) obtained in both measurement modes are presented in comparison with transmission data (1 eV step) of a 12 μm Cu-foil extracted for the CARS database of XANES spectra [13].

The application of XANES methodology reaches optimum sensitivity when the excitation geometry are carefully adjusted to maximize the fluorescence signal of the analyte element and to reduce spectral background. This can be achieved by the various alignment degrees of freedom offered by the sample manipulator that allows setting a sample in external total reflection geometry. Using for example, a 9-stage May-type cascade impactor with adjustable sampling air volume capacity per stage, collection of size fractionated airborne particulate matter down to 0.07 μm equivalent aerodynamic diameter can be achieved directly onto 20×20 mm^2 Si wafers. The air particulates are deposited in a form of a stripe with 200–500 μm width for each stage. This deposition geometry is ideally suited to TXRF using synchrotron radiation, since the small vertical dimension of the beam (260×130 μm^2) allows the full illumination of the aerosol deposit [14,15]. Three alignment procedures were performed before carrying out energy scan measurements at optimized excitation conditions: At first, the incident angle was adjusted below the critical angle for external total reflection of the exciting X-ray beam (by choosing an incident energy just above the Zn-K edge), determined as the inflection point of the Si-K XRF intensity profile versus incident angle. Secondly, the ϕ polar axis sample allowed adjusting the stripe of deposited aerosol particles parallel to the direction of the exciting beam, whereas for the final alignment, the sample stage that it is perpendicular to the horizontal plane (X axis coordinate) was utilized so that the incident beam (vertical size of about 130 μm) to scan vertically the aerosol deposit and identify the

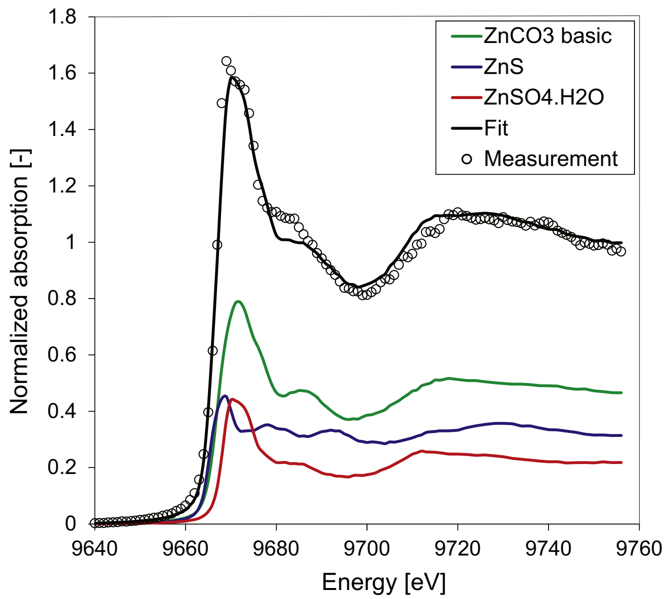

Fig. 5. Evaluation of a Zn K-edge TXRF-XANES spectrum recorded for a 0.18–0.3 μm fraction of airborne particulate matter originating from burning of painted wood with linear combination of standard spectra.

maximum Zn-Kα intensity. Through this experimental procedure, the optimum (θ, ϕ and X) angular and spatial coordinates could be specified for a particular sample and analyte of interest. As an example, a XANES profile across Zn-K edge obtained in TXRF detection mode with 1 eV step with 10 s acquisition time per step is reported in Fig. 5 corresponding to a 0.15–0.3 μm fraction of an aerosol sample originating from the burning of painted wood. The total deposited mass of Zn was as high as 84 ng, calculated based on a TXRF spectrum recorded at 10 keV excitation energy. The XANES data were processed by ATHENA tool [16] applying a self-absorption correction as proposed in [15]. Reasonable fitting based on a linear combination of standard XANES spectra revealed that Zn was present mostly as $ZnCO_3$ (47%) and ZnS (32%) with lesser extent of $ZnSO_4$ in the submicrometer aerosol particles originating from burning of painted wood. The difference between the fitting and the experimental XANES spectra are mainly due to the fact that additional Zn compounds might be present in the particulate matter sample [17]. For further refining of the fitting results additional standard samples of different chemical forms of Zn are required.

5. Conclusions

This work describes a custom made functional binding of a LabVIEW GUI with Tango control system. The software development aims to support data acquisition at the newly developed synchrotron beamline IAEA end-station at Elettra Sincrotrone Trieste allowing a flexible, optimum and combined application of various X-ray spectrometry based analytical methodologies such as different XRF variants, XRR and X-ray absorption spectroscopy measurements.

The XRF beamline and IAEA end-station is currently utilized through the IAEA-Elettra Sincrotrone Trieste collaboration agreement and under the IAEA Coordinated Research Project (No. G42005, "Experiments with Synchrotron Radiation for Modern Environmental and Industrial Applications", 2014-2017) for research in materials science (characterization of nano-structured materials, dopants in semiconductors), in biology (study of essential or toxic elements in plants in relationship with biofortification, phytoremediation and phyto-mining techniques), in biomedicine (Bio-sensing technologies and nano-medicine design, role of trace elements in humans), in the characterization of trace elements in environmental samples, technological studies of ancient materials and in the development of novel conservation materials.

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