

VIBA-Lab 3.0: Computer program for Simulation and Semi-quantitative analysis of PIXE and RBS Spectra

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Abstract

VIBA-Lab is a computer program originally developed by the author and co-workers at the National University of Singapore (NUS) as an interactive software package for simulation of Particle Induced X-Ray Emission (PIXE) and Rutherford Backscattering Spectra (RBS). The original program is now being redeveloped to a VIBA-Lab 3.0 in which the user can perform semi-quantitative analysis by comparing simulated and measured spectra as well as simulate 2D elemental maps for a given 3D sample composition. The latest version has a new and more versatile user interface. It also has the latest data set of fundamental parameters such as Coster-Kronig transition rates, fluorescence yields, mass absorption coefficients and ionization cross sections for K and L lines in a wider energy range than the original program. Our short-term plan is to introduce routine for quantitative analysis for multiple PIXE and XRF excitations.

The VIBA-Lab software package is an excellent teaching tool for students and researcher of PIXE and RBS techniques. At the same time the program helps when planning an experiment and when optimizing experimental parameters such as incident ion energy and species, detector specifications, filters, geometry, etc. By "running" a virtual experiment the user can test various scenarios until the optimal PIXE and BS spectra are obtained and in this way save a lot of expensive machine time.

Key words: PIXE, RBS, Nuclear Microscopy, simulation, data reduction

Introduction

Ion Beam Analytical (IBA) techniques and in particular, Particle Induced X-Ray Emission (PIXE) and Rutherford Backscattering Spectrometry (RBS) are utilized by many laboratories for elemental analysis and concentration depth profiling of a wide variety of materials and elements. Because of that, there was a high demand for precise quantitative analysis which in turn resulted with intense research activities related to understanding ion beam interaction with matter. Theory is now well understood and most of the fundamental data sets required to simulate IBA interactions with matter are well known. A number of dedicated computer programs for quantitative analysis was developed by various IBA groups, as for example: GEOPIXE [1], GUPIX [2], PIXAN [3], WINDF [4], to mention only several, the most popular codes.

However, none of these codes is dedicated to simulate PIXE and RBS spectra. To fill that niche, we developed VIBA-Lab which, to the best of our knowledge, is still the only computer code that can, at the same time, simulate PIXE and RBS spectra for any given geometry and sample composition.

In the latest versions, the code is extended with added simulation of Nuclear microscopy elemental maps for a given 3D elemental composition of the sample. Also, a new routine for comparison of measured and simulated PIXE spectra and for semi-quantitative analysis is added in Java script.

In the following sections, a brief description of major VIBA-Lab 3.0 features is given.

1. The VIBA-Lab 3.0 computer code

1.1 Graphic user interface: defining Experimental Parameters

The VIBA-Lab is written in Borland C++ and the Object Windows Library (OWL) as object-oriented framework designed for Windows applications. The program is based on the TPIXAN code initially developed by the author (I. Orlic) for quantitative PIXE analysis [5]. The code was later translated to C++ and a new graphic user interface (GUI) introduced. Program was renamed to Virtual Ion Beam Analysis or VIBA-Lab for short with the aim to be an integrated, easy to use computer code that enables IBA researchers to perform simulation of both PIXE and RBS spectra for a variety of incident ions and for a wide range of experimental parameters [6, 7, 8, 9].

User can define experimental parameters of all major components either through the pull down menus or by clicking on dedicated icons. The following parameters can be changed through interactive dialogs:

- * **Accelerator parameters:** parameters such as ion species (protons, deuterons and He ions are implemented in the current version) in the energy range from 0.1 to 10 MeV.
- * **PIXE and RBS detectors:** to be able to simulate detector efficiency, full description of all detector parameters are required; crystal thickness and active areas, thickness of Au and dead layers, angle of incident ions and angles of emergent X-rays and BS ions, etc. Further, four commonly used filters (kapton, mylar, Al and Be) can be selected in addition to a user-defined filter. The user can define filter thicknesses and the diameter of the central hole when using so-called 'magic' filter. An example of dialog box for defining detector and filter parameters is given in .

- * **Sample layers and composition:** sample can be subdivided in up to 10 uniform and homogeneous layers and each layer can have up to 10 elements. Relative concentrations can be defined as atomic mass ratios or as weight fractions. Periodic table is provided for user's convenience so it is relatively easy to add elements and their concentrations into each layer.
- * **3D Sample composition and inclusions:** the latest version was further improved by adding simple 3D objects (ellipsoids and rectangular prisms) into the scanning field so that 2D elemental maps can be simulated.
- * **Output:** simulated PIXE and RBS spectra are displayed together with measured spectra, residuals, 2D elemental maps, auxiliary functions needed for optimization of experimental parameters. They can be saved as bitmaps or in text formats.

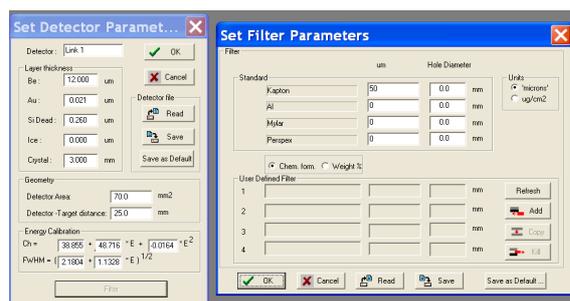


Figure 1 Through a simple GUI user can define all detector parameters; crystal thickness and active areas, thickness of Au and dead layers, angle of incident ions and angles of emergent X-rays, energy calibration as well as all filter parameters.

1.2 Simulation of PIXE spectra and 2D elemental maps

In VIBA-Lab, simulated X-ray yields are calculated by means of a number of sub-routines that include major physical processes involved in X-ray production and attenuation. The algorithm employed is already described in our previous work [5,6,7,8] and only brief account is given here. Initially, sample is divided into a number of 'thin' slices and the total X-ray yield is calculated by summing-up yields emerging from individual slices. Yields are further corrected for the absorption in the sample, for the absorption in the filters and for detector efficiency.

In the current version of the program introduced is a simple semi-quantitative analysis based on comparison between simulated and measured spectra. Simulated and measurement spectra together with the residual plots are shown in a browser. User can zoom in, change the X and Y scale, recalibrate energy for the measurement or change from linear to logarithmic scale.

An example of such comparison is given in .

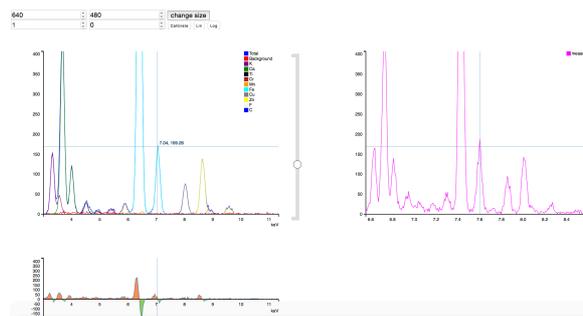


Figure 2 Through a modern Java interface user can perform semi-quantitative analysis based on comparison between simulated and measured spectra. One can zoom-in and out X and Y scale, change from linear to log scale and change concentrations of individual elements until good agreement is achieved. On the above figure, measured aerosol spectrum (b) is compared with the simulated spectrum (a) and the difference is shown as residuals (c).

To be able to calculate simulated X-ray yields, a number of fundamental atomic parameters are required. In VIBA-Lab 3.0 the following data sets are adopted:

a) Ionization and production cross-sections

In the VIBA-Lab, the ionisation cross sections (ICS) are calculated by using ECPSSR [10] approximation and the code developed by our group [5]. As the ECPSSR theory does not perfectly reproduce experimental cross sections, the obtained theoretical ICS values are multiplied by an empirical, so called S function. In the case of proton excitations of K shells, the S function provided by H. Paul [11] is implemented while in the case of the L-shell excitation the S functions obtained by I. Orlić is used [12]. In this way, the error introduced in calculated ICS is estimated to be between 2 and 4% [12]. For all other incident ions theoretical, ECPSSR cross sections are used.

b) Koster-Cronig rates, fluorescence yields and branching ratios

In order to calculate x-ray yields, ionization cross sections have to be transformed to the corresponding production cross sections. For this purpose, the fluorescence yields given by Krause [13] and the recent recommended values of I. Campbell [14] are used. Branching ratios for K shell are from the Khan and Karimi's work [15] and the intensities of the individual L X-ray lines are from the work of D.D. Cohen and M.Harrigan [16]. As relative line ratios are functions of the incident ion energy, the ratios in between tabulated values are obtained by means of the linear interpolation in the log-log scale.

c) Mass attenuation coefficients

To facilitate fast calculation of mass attenuation coefficients (MAC) the semi-empirical scheme developed by I. Orlic et al. [17] is used. The scheme is applicable for all elements and in the entire photon energy range between 0.1 keV and 1000 MeV. Accuracy is estimated to be 2-3% in the entire energy range, except at the immediate vicinity of the absorption edges and at the energies below 1 keV where, due to experimental database uncertainties, errors are somewhat bigger.

1.2.1 Simulation of bremsstrahlung

To make simulated PIXE spectra as realistic as possible continuous PIXE background (so called bremsstrahlung) and statistical noise are simulated as well. For that purpose, the semi-empirical algorithm published by K. Murozono et.al [18] is used. Simulated bremsstrahlung is superimposed on simulated X-ray yields and the random statistical noise.

1.2.2 Simulation of 2D elemental maps

In the latest versions of VIBA-Lab a unique feature is added: an algorithm for generating elemental maps from a given 3D sample composition. This routine is designed to enable Nuclear microscopy researchers to study how the size, shape and composition of various inclusions influence the X-ray yield and artefacts often visible in 2D elemental maps. Introduction of this routine required major change of the original code, especially in terms of code optimisation, as simulation of 2D elemental maps is computationally very intensive. Also, to allow a user to define a 3D-sample composition, more advanced "drag and drop" object oriented routines are developed. The algorithm used to calculate 2D elemental maps is described in more details in our previous work [19]. The program allows users to define 3D inhomogeneous thick targets in terms of slices, inclusions and voids all with different compositions. An example is given in Fig. xx. User can choose scan areas of 5, 10 or 25 micrometers and initiate the area or line scan. The resulting elemental maps or intensity line profiles are displayed on the screen and can be saved as bitmaps or text files, see Fig. xx.

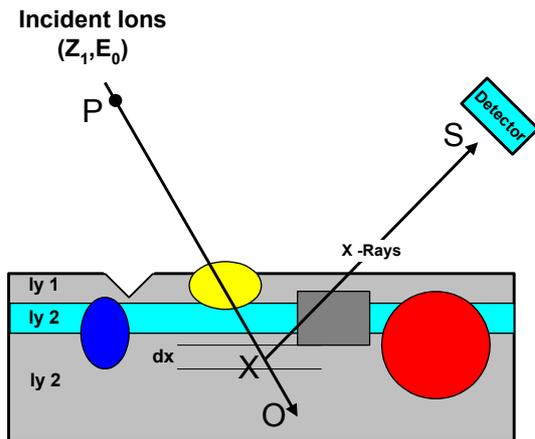
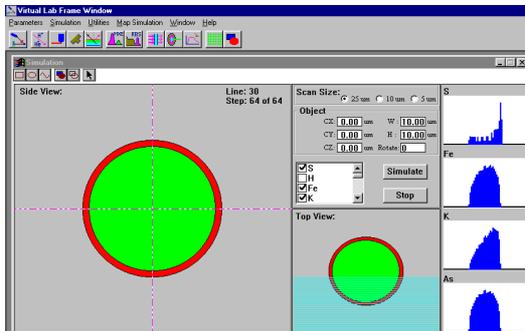


Figure xx



1.3 Simulation of RBS Spectra

The algorithm used to simulate RBS spectra is the same as the one employed in the program RUMP. Details of calculations can be found in the original work by L.R. Doolittle [1??] and all additional features are described in the work of

K.K. Loh [7??]. To improve BS fitting for low Z elements the current version also contains non-Rutherford cross sections for proton scattering from light elements (O, N, C and Si) at three different scattering angles, i.e. 110°, 150°, and 170°. To calculate non-Rutherford cross sections at different proton energies, Breit-Wigner's formula and the coefficients provided by the Amirikas et al. [20] are used.

This routines for calculating the stopping cross section are based on the Ziegler's compilation [21] which provides stopping cross-section for all ions in any elemental solid target for incident energies up to 100 MeV/amu.

1.4 Output and the Auxiliary routines

Once the simulation of PIXE and/or BS spectra is completed, the resulting spectra are displayed on the screen. The user can either save the spectra as bitmaps or as text files for later processing. Optionally, the user can change some of the experimental parameters and run the simulation again. To see the effect of the change, the new spectrum can be overlapped with the previous one.

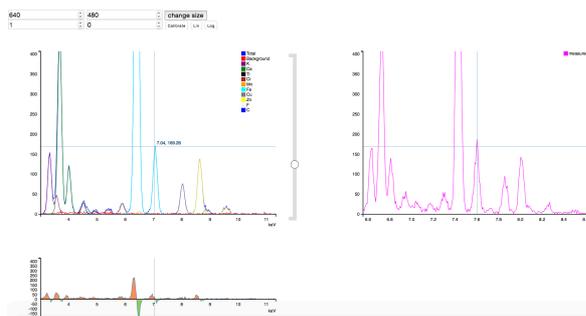
Besides providing visual presentation of the simulated spectra, the user can save a table where the absolute and relative PIXE yields of all X-ray lines of interest (K and L) are listed individually for each layer as well as the estimated limits of detection (LOD) which is calculated by using the usual 3 standard deviations of the background counts under the X-ray line of interest (within 1 FWHM).

VIBA-Lab has a number of auxiliary computer codes for easy calculation of various physical parameters relevant to PIXE and RBS techniques. These parameters are: mass attenuation coefficients, K and L shell ionization and production cross sections for proton, deuteron and He ion impacts, elastic and inelastic scattering cross sections, energy loss for various incident ions, and Si(Li) detector efficiency. As for the main simulation routines, each of these auxiliary programs provides two forms of output: on-screen graphics and the table that can be saved as a text file. More detailed description of these routines is given in our previous work[8, 9].

2. Work in progress and future plans

As mentioned earlier, VIBA-Lab is currently undergoing major restructuring. The new version will allow the user to perform quantitative analysis, firstly for the broad beam geometry and in the later phase for the nuclear microscopy.

New developments of the VIBA-Lab program builds on the existing code base consisting of approximately 100k lines of code over 265 source files written in an obsolete Borland C++. We are therefore undertaking a major code refactoring. Routines that contain physics are being untangled from the existing code base and converted to Java programming language with the aim to be portable across all major platforms.



Conclusion

The computer code VIBA-Lab was initially developed for simulation of PIXE and RBS spectra basically with educational aim in mind. In the latest versions added are two new features: semi-quantitative analysis based on comparison of measured and simulated PIXE spectra as well as simulation of elemental maps. The program allows the user to define important experimental conditions and then simulate PIXE and RBS spectra for any sample and excitation conditions.

VIBA-Lab is very useful in two ways: firstly, it is an excellent teaching tool for students/researchers with no experience in PIXE/RBS techniques. Secondly, it is of immense help in planning an experiment and choosing the optimal experimental conditions for various analytical problems that PIXE analyst encounter in contacts with various collaborators. With the use of VIBA-Lab one can run a simulated experiment for an unknown sample and test various settings/scenarios to achieve optimal results without actually running the experiment. This can potentially save a lot of expensive machine time that would otherwise have been spent on trial and error experiments.

We are currently undertaking a major code refactoring. C++ code is being converted to Java programming language with the aim to have a code that is portable across all major platforms. The new version will be a modern, modular, multi platform program that will run on all major operating systems; Windows, MacOS and Linux.

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