Allegria: a new interface to the ERD program

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Abstract

As a new PC-based acquisition system has been installed to replace the VAX-based system of the elastic recoil detection by time-of-flight (ERD-TOF) and gas-counter ERD setups at University of Montréal, a new analysis software has been developed. It includes a calculation of the energy calibration involving pulse height defects corrections for each element. It has been further improved to process a number of different ERD or Rutherford backscattering spectrometry (RBS) spectra in a single run and now incorporates stopping power calculations based on SRIM-2003 parameters. The application comes with a graphical interface that is used to extract mass separated spectra from event-list files. A second application allows the user to input the experimental parameters and prepares a command file that is passed to the ERD program. The latter iteratively converts the energy spectra into depth profiles for each mass. Resulting atomic fractions are normalized to one of the elements, typically the substrate or one of its components. Some examples of analysis for both TOF and gas counter ERD measurements are presented and discussed. The program and source code will be made available to the ion beam analysis community under GNU licensing conditions.
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1. Introduction

Probably every Ion Beam Laboratory of importance has developed its own software for data analysis. A few of them have gained widespread popularity, such as simulation programs RUMP [1], SimNRA [2] and RBX [3], or more limited but still significant cross-laboratory usage such the spectrum-to-depth-profile converter Allegria [4]. Others, like DataFurnace [5], have reached a high degree of sophistication in solving complex RBS spectra. The process is somewhat simpler when the spectra are obtained with methods like elastic recoil detection (ERD), where the different components of the signal are readily separated from the beginning.

As a pioneer in the domain of ERD, the Ion Beam Laboratory of the Université de Montréal has also developed and continuously improved its own code over the years. With the invention of the elastic recoil detection analysis (ERDA) technique by L'Écuyer et al. in the 70s [6], an analysis program named ERD was setup in order to convert the measured spectra into depth profiles. Initial

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versions calculated energy-to-depth correspondence tables that were then used to convert the energy axis into a depth scale. Iterative procedures were developed to correct the stopping power according to Bragg's rule [7,8]. With the creation of the first time-of-flight (TOF) based ERD system in the 80s [9], a complete software was deployed that not only converted the spectra but also helped to analyse the resulting profiles and manage the information efficiently [10]. A drawback was that this software was intensively using VAX-VMS specific routines no longer implemented on current commercial systems. The core of the package, the ERD program, was still portable and implemented with several interesting features such has pulse height defect (PHD) calculation for the correction of the energy calibration of each mass in a surface-barrier detector.

2. ERD profiling program

In order to establish the depth profile of each element, the ERD program calculates the energy loss of the projectile and the recoiled atoms for small depth intervals. For each spectrum, it then calculates the number of counts in the energy intervals corresponding to each depth interval and deduces the concentration. During iteration zero, for energy loss calculation purposes, it assumes that the target is entirely made of a single element, identified by the user as the ''monitor''. During each subsequent iteration, the program uses the Bragg's rule to estimate the energy loss, considering the concentrations found in each depth interval during the previous iteration. It also takes into account the energy loss of each detected atom through a timing foil or absorber. As mentioned above, the program also includes a calculation of the energy calibration for each element based on PHD calculations [11], which is useful since heavy ions are involved. In this case, only the slope of the α-particles calibration for the detector is required. The user may also specify a two-parameter calibration. Depth units are either in $\mu g/cm^2$ or in at/cm^2 and energies in keV.

Among many internal improvements, the new version of the program now relies on SRIM 2003 stopping power tables [12]. It can also more easily operate with ERD or RBS spectra obtained on different setups, that is, with different energy calibrations, scattering angle, solid angle, etc., as long as each spectrum involves only one element.

3. SpectrumExtractor program

The purpose of this program is to read an event list file generated during the measurement, each event containing multiple detection channels, and to display them in such a way that the user can extract from the data the energy spectrum of each element. The user can display different channel combinations on each axis. Fig. 1(a) gives an example of a measurement made on a SiO_2 layer using gas-counter ERD with a 50 MeV Cu beam [13]. The horizontal axis represents the signal collected on the last electrode of the detector (ΔE_{rest}), while the vertical axis represents the sum of the signal collected on the first two electrodes ($\Delta E_1 + \Delta E_2$). Each element can be identified by a polygon, whose coordinates are recorded for future uses. The user can select more complex display options as illustrated in Fig. 1(b). The measurement presented in (a) was actually made with a mask containing a hole lattice and placed in front of the gas-counter ERD. The bottom electrode of the detector is divided in a backgammon pattern. The horizontal axis of the graph represents the ratio $(a - b)/(a + b)$ where channel a and b are the charge collected on the left and right bottom electrodes, respectively. For the vertical axis, the same ratio is used but with a and b channels representing the charge collected on the top and bottom electrodes, respectively. This is essential information to carry out kinematics corrections later during the analysis, as the square lattice appears somewhat distorted.

To help users with ERD-TOF spectrum extraction, the plot can be reshaped to display the mass on the vertical axis. Fig. 2 gives an example for a glass sample analysed by ERD-TOF with a 30 MeV Cl beam. The left part of the figure shows the time-of-flight t as a function of energy E, while the right part shows the mass m against energy.
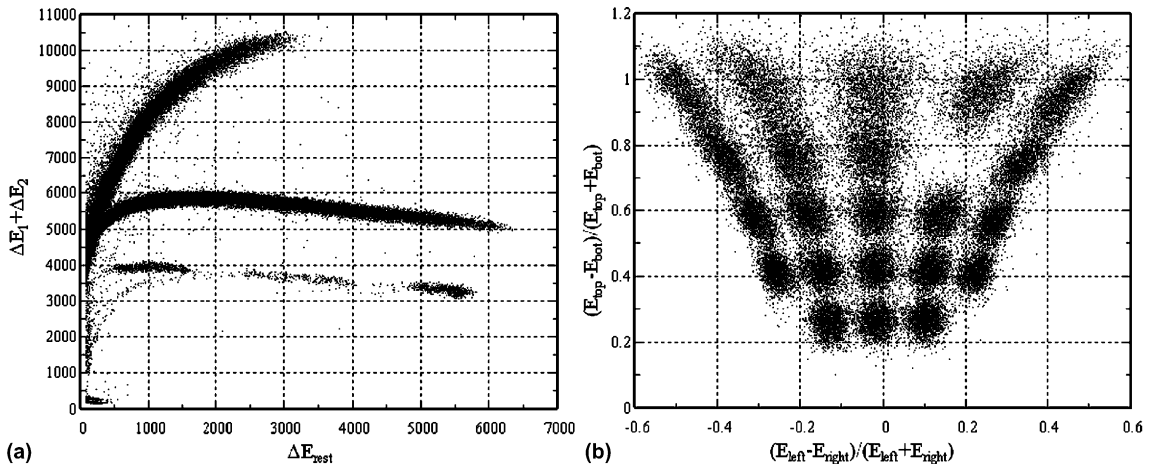
Fig. 1. Gas-counter ERD spectrum on a 528 nm layer of SiO_2 on Si, measured using a 50 MeV $^{63}Cu^{9+}$ beam. (a) Signal from the first two electrodes ($\Delta E_1 + \Delta E_2$) plotted against the signal from the third electrode (ΔE_{rest}) showing the detected Si, O and C recoils; (b) top–down versus left–right electrodes signals for the oxygen recoils. The spot pattern is due to the presence of a mask with a square hole lattice in front of the detector.
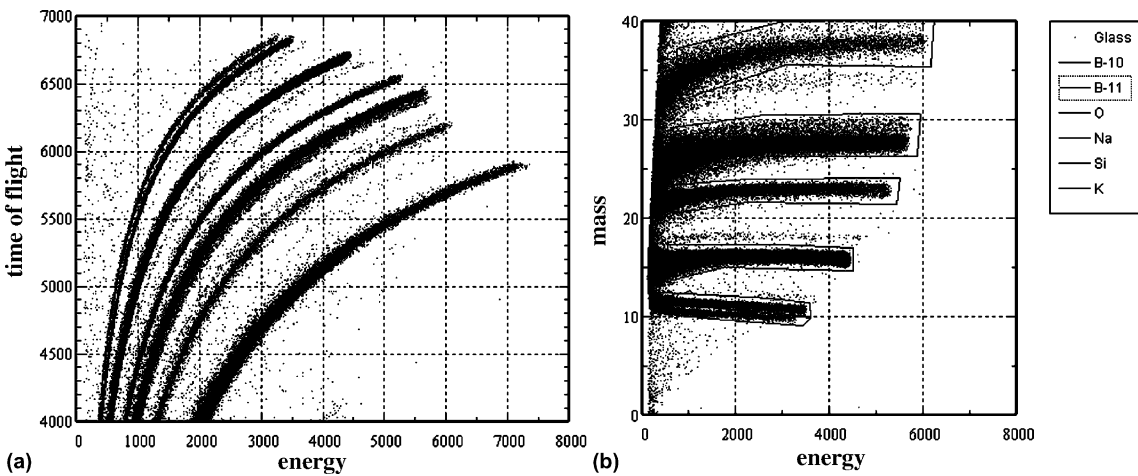

Fig. 2. ERD-TOF spectrum of a glass sample containing ^{10}B, ^{11}B, O, Na, Si and K, measured using a 50 MeV $^{63}Cu^{9+}$ beam. (a) Time-of-flight against energy; (b) vertical axis reshaped to display mass versus energy, where the main constituting elements are identified by polygons.

The mass is calculated according to the following expression:

$$m = 2(E - E_0)(t_0 - t)^2/l_0^2,$$

where E_0, t_0 and l_0 are parameters associated with the zero in energy calibration, the delay in the TOF measurement, and the camera length, respectively. These parameters are actually adjusted so that a given mass will appear as a hori- zontal stripe on the display. Since a single set of parameters is not suitable for all masses, dif- ferent sets can be saved and recalled later by the user.

A spectrum can also be generated by accumu- lating the events of a given channel in the event list file if, for example, this channel represents the signal coming from a simple surface barrier detector.

Once the elements are identified by different polygons, the data can be projected on an energy axis. This energy axis does not need to be one of the axes of the plot, which are really used to differentiate the elements. The resulting spectra will appear in another window where the user can make other operations on the spectra, such as subtracting background.

4. Allegria

Allegria, now spelled with two "*l*" to distinguish from its predecessor, is actually an interface to the ERD program described above. A dialog helps the user to set experimental parameters, select the detected elements and set related detection parameters, including the analysis method (ERD or RBS) and the spectrum file. Once the parameters are set, they are passed to ERD that makes the iterative conversion. Allegria then reads back the resulting profiles. Functions are provided to save the data in a single, multi-column file or in separate files. As an example, Fig. 3 shows the depth profiles obtained from the data in Fig. 2.

The program operates in such a way that the user must keep all the files corresponding to a target in a given directory. The parameter file passed to ERD is saved together with the depth profiles so the user can easily retrieve the parameters associated with different experiments.
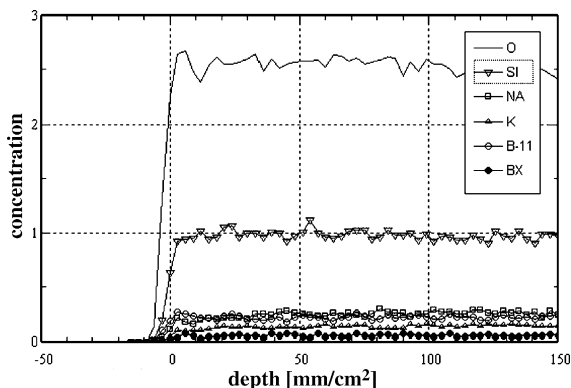

Fig. 3. Depth profile of the elements identified in Fig. 2(b). The concentrations are normalized to the Si profile.

5. Program distribution and computer requirements

The package, including sources, is distributed under GNU licensing conditions. It namely means that all other programs using parts of this code also have to be distributed under the same condition and must retain the copyright notice accompanying each file. The graphical user interface has been developed in C++ using Trolltech Qt 2.3 and should compile on any supported platform including Linux and Windows. The program is available for download from the web site of the first author. [1]

In terms of computation requirements, the most demanding part of the package is the SpectrumExtractor program that has to manage and display event list files containing hundreds of thousands of events. As a rule of thumb, to operate smoothly, the processor speed must be of the order of 1 kHz per event.

6. Summary

Based on existing programs, a new software has been developed in order to extract energy spectra from multi-parameter ERD detection systems and iteratively convert them into depth profiles. The SpectrumExtractor program is flexible and can be easily modified for the purpose of specific applications. The "conversion engine" is implemented with several useful features such as PHD calibration correction and now relies on SRIM 2003 stopping power calculation. The program runs on a PC on various platforms and is distributed free of charge to the IBA community.

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[1] Author's web site: www.lps.umontreal.ca/~schiette.

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