PAMPA Tutorial

1 Introduction

PAMPA (Parameter Assessment Method for PIXE Analysis) is a software package for the analysis of x-ray spectra induced by proton impact (PIXE). The program is based on a method for optimizing atomic parameters related to the elements present in the target, parameters related to the sample, and instrumental parameters.
The software is written in Object Pascal, and runs under Linux and Windows operative systems. PAMPA has a graphical environment developed with the Lazarus IDE tool. Within this environment, the sample characteristics and the parameters to refine can be chosen.

The program allows the analysis of two kinds of samples: thick (bulk) sample and film on a bulk substrate. The analyzable elements range from B to U, involving up to 30 elements per analysis. The present version of PAMPA allows up to 30 K or L lines for each element to be analyzed.

Regarding the ionizing beam, protons in the whole range of interest in PIXE are considered, since the data bases used for both ionization cross section and stopping power are recommended between 10 keV and 10 GeV.

2 Installation

2.1 Needed software

To use PAMPA in Linux the following software packages must be installed:

- Lazarus, fpc, fpc-src: http://www.lazarus-ide.org/index.php?page=downloads
- Gnuplot: http://www.gnuplot.info/download.html

For the Windows version only Lazarus must be installed:

- Lazarus: http://www.lazarus-ide.org/index.php?page=downloads

2.2 File structure

Within the main PAMPA directory there are the following subdirectories:

- dat : Involves the data bases used by the program.
- esps : Involves the files .spe which consists of the experimental spectra. Two example spectra corresponding to a bulk sample and a thin film supported on a substrate are included in the installation package.
- pampa : Involves the program files.
- pampa/ajustes: Involves the input files included in the installation package as examples of thick sample (mgruesa.dat) and thin film (mdelgada.dat) corresponding to the example spectra included in 'esps' directory.

2.3 Installation process

To compile the software package, the following steps must be carried on:

- Open the 'pampa.lpr' project with Lazarus.
- In the 'Unit1.pas' file set SistOp:=1 for Linux and SistOp:=2 for Windows. Set the 'DiUser' variable as the directory where the programa was copied.

3 Structure of input files

3.1 Spectra

The files containing spectra must have the extension '.spe' and the structure shown bellow, where in the second line the inicial and final channel numbers are displayed; the subsequent lines correspond to the number of counts for each channel, with 10 values in each line.
In 'pampa' directory, the program 'PIXtoPAMPA.pas' converts a '.PIX' file involving four columns, to the format used in PAMPA. This routine is given just as an example that should be modified for each particular spectrum file format.

```
$DATA:
      0    2048
       0       0       0       0       0       0       0       0       0       0
       0       0       0       0       0       0       0       0       0       0
       0       0       0       0       0       0       0       0       0       0
       0       0       0       0       0       0       0       0       0       0
       0       0       0       0       0       0       0       0       0       0
       0       0       0       0       0       0       0       0       0       0
       0       0       0       0       0       1       2       3       2       2
       2       2       1       0       0       0       0       4      14      11
      15      13      11      22      42      99     170     452     672     894
    1114    1929    4140    6520    7166    7055    8308   16479   33292   47591
   42243   23224    9326    2687     775     471     385     443     387     425
     399     440     433     458     489     477     502     475     519     509
     501     609     555     527     463     406     475     483     491     428
     477     517     529     542     611     738     810    1002    1189    1308
    1778    2348    2877    2951    2583    2378    2503    4832   13036   28942
   52475   68955   70918   59271   44086   28755   16286    9250    5069    2465
    1130     549     319     286     290     402     455     488     458     366
     332     265     257     226     193     163     148     115     103      91
      83      99      84      77      80      81      61      86      67      68
      61      59      62      56      58      51      51      57      58      46
      37      38      43      47      53      40      37      45      37      35
      41      32      28      44      36      28      32      33      20      32
      25      42      35      49      66      78      94      76      84      54
      51      38      31      19      15      25      12      18      18      18
      14      17      14      11      18      12       9       9      11      12
      10      11      15      10      14      11      11      11      19      19
      19      11      11       9       9      10       5      11      17       8
       6       9      14      13      23      21       9       9       8       5
       6      11       4       9       6      13       7       9      10      10
       8      11       9       3       9      12      12      15      14      14
       4      11       8      10       7       4       2       7       5       4
```

3.2 Input configuration files

The input configuration file has an extension '.dat' and involves all the information related to the analyzed sample, along with all the optimizable parameters. Each parameter has two associated variables: 'Código', which defines if the parameter will be refined (Código=1) or not (Código=0), and 'Lambda', which corresponds to a fraction of the associated parameter (0.1 for default). 'Lambda' defines the searching distance for each parameter in the minimization algorithm.
The configuration file can be created by inputing all the required information in the different windows of the program, or a previously created configuration file can be used. In the last case, the file must be open through File→Open.
To open one of the '.dat' example files provided with PAMPA it is necessary to edit it and change the directory where the corresponding spectrum was copied.

4 Optimization procedure

The parameters to refine must be chosen by means of the check-boxes, defining a value for the convergence tolerance and the spectral region to fit.
When the fitting process ends, the program updates the refined parameter values and, thorough the Gnuplot environment, displays a plot of the experimental spectrum, along with the fitted curve and the residuals. In addition, each contribution of continuous background, characteristic peaks, their asymmetric tails, and spurius peaks are displayed separately.
By means of File→Save , the '.dat' file is saved together with a '.sal' file, which contains: the experimental spectrum, the fitted curve, the continuum, the characteristic lines, the asymmetric tails and the sum peaks.

4.1 Refinable parameters

The parameter that can be refined during the minimization procedure are the following:

- Calibration: Gain (G) and Zero (Z_0).
- Detector characteristic thicknesses: window, ohmic contact, dead layer.
- Countinuous background: A, B and C.
- Detector response: *Noise* (n) and Fano (F).
- Global scale constants: K- and L-line group constants.
- Characteristic energies and relative transition probabilities.
- Peak asymmetric tails: β_{jq} and t_{jq}.
- Mass concentrations of the elements present in a bulk sample (layer 1).
- Mass concentrations of the elements present in a thin sample (layer 2).
- Sum peaks: I_{suma}, b and w.
- Intensity of the internal Si fluorescence.