1. NAME AND TITLE OF DATA LIBRARY

PIXE2010: Proton/alpha Ionisation (K, L, M shell), Tabulated Cross Section Library.

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAMS

IONXSEC: auxiliary software to print out data.

3. CONTRIBUTORS

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4. HISTORICAL BACKGROUND AND INFORMATION

The physics aspects associated with PIXE involve the creation of a vacancy in the shell occupancy due to ionization, and the emission of X-rays from the following atomic de-excitation.

Various theoretical and empirical models are available in literature to describe ionisation cross sections for different interacting particles, as well as compilations of experimental data.

The *PIXE2010* data library is based on the developments described in [1]: it provides tabulations of ionisation cross sections for proton and α (alpha) particle impact as a function of element, atomic (sub-)shell, and incident particle kinetic energy, for elements with atomic number from 1 to 92.

This data library derives from software developments meant for use with the Geant4 [2] simulation toolkit; nevertheless, the data library itself is independent from Geant4 and can be used in other software environments.

Cross section values at a desired energy can be calculated by interpolation over the tabulated values.

5. APPLICATION OF THE DATA

The data can be useful to Monte Carlo simulation of PIXE or software systems for elemental analysis.

6. SOURCE AND SCOPE OF THE DATA

The data library contains cross section tabulations for K, L and M shell ionisation based on various theoretical and empirical models. The models from which the data derive are described in detail in [1]; the most relevant related references are cited next to the models.

The cross sections associated with each model have been pre-calculated either using existing software documented in literature (ISICS [3] for the ECPSSR model and its

variants), or developing ad hoc code.

Theoretical cross section models include:

1. Plane Wave Born Approximation (PWBA) [3]
2. ECPSSR [4]
3. ECPSSR with United Atom correction (ECPSSR-UA) [3]
4. ECPSSR with corrections for the Dirac-Hartree-Slater nature of the K shell(ECPSSR-HS) [5]
5. ECPSSR with improvements to K shell cross section specific to high energy(ECPSSR-HE) [6]

The tabulations corresponding to theoretical calculations span the energy range between 10 keV and 10 GeV. ECPSSR tabulations have been produced using the ISICS software [7], [8], 2006 version and an extended version [9] including high energy developments.

Empirical cross section models for K shell proton ionization include the tabulations for protons documented in [10] and a more recent one [11]. An empirical cross section model for K shell ionization by α particles is based on the tabulations in [12]. Empirical cross sections for L shell ionization by protons are based on models by Miyagawa et al. [13], Sow et al. [14] and Orlic et al. [15]. The empirical models are tabulated consistently with their energy range of validity.

Details about the accuracy of the cross section are reported in [1]; specifically, section V (pp. 3627-3639) is devoted to the verification and validation of the cross section models tabulated in the data library.

Copies of [1] can be downloaded from http://ieeexplore.ieee.org/xpls/abs_all.jsp?arnumber=5341442 or can be requested from the contact person indicated in Section 3.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAM

Data retrieval program "IONXSEC" is included in the package. The IONXSEC code may be used to print-out the PIXE2010 data, according the following options:

- choice of the element;
- choice of the impinging particle (alpha or protons);
- choice of the shell: K, L (L1, L2, L3), M (M1, M2, M3, M4, M5);
- choice of several proposed models for each shell;
- choice of the energy range.

Instructions about how to install and run the program can be found in the README file in the "ionxsec" folder.

8. DATA FORMAT AND COMPUTER

Data are stored in files, which make up a data library for PIXE simulation. Each cross section data set is stored as a separate file.

The library is provided in computer independent ASCII format, which allows the data to be easily transported between computers. The entire library requires approximately 22 MB of storage.

The data are divided in two main folders: a) proton Folder, b) alpha Folder.

Each of these folders contains:

a) **k** folder;   it contains a folder for each implemented model for K-shell ionization
b) **l** folder; it contains a folder for each implemented model for L-shell ionization
c) **m** folder; it contains a folder for each implemented model for M-shell ionization

Each model folder directory contains an ASCII file for each element; it appears as two columns listing energy values and corresponding cross section values. Energy and cross sections are given in MeV and mb, respectively.

9.   TYPICAL RUNNING TIME
Few seconds to print the whole set of cross sections.

10.   REFERENCES

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11. CONTENTS OF LIBRARY
The ASCII data files are approximately 22 MB. The document mentioned in Section V is also included.

12. DATE OF ABSTRACT
September 2010.

13. KEYWORDS:
PIXE, Ionization, cross section, X-ray