Common Data Processing System Version 5

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Since 1989, we have been constructing the spectral data processing system named Common Data Processing System (COMPRO) under the VAMAS (Versailles Project on Advanced Materials and Standards) umbrella. COMPRO can be downloaded from the web site (sekimori.nrim.go.jp) and runs on Windows. The main objectives of COMPRO are to provide a tool for sharing spectral data and a common bed for data processing procedures proposed by scientists. COMPRO has been upgraded 5 times and the present version is 5.4. The objective of the paper is to introduce the latest version of COMPRO.

1. Introduction

About 25 years have passed since commercial AES and XPS apparatuses appeared. Since that time, spectral data for different surfaces have been obtained by many scientists and engineers. However, almost all of them were not shared and not stored as databases. Nowadays, it becomes important to stock these knowledge or data as databases, because we aware that these data are very useful to characterize unknown surfaces. To create a spectral database, we have to establish a system to share spectral data taken on different machines.

Since 1989, we have been constructing the spectral data processing system under the VAMAS (Versailles Project on Advanced Materials and Standards) umbrella [1,2]. This system is called Common Data Processing System (COMPRO). COMPRO is designed as a program to convert an original spectral data file to one with a common structure [3], to assess the data processing procedures proposed by scientists, to calibrate energy and intensity scales, to check a spectrum, to check the reliability of the data processing algorithms proposed by scientists, and to build both spectra and physical properties databases. In this system, the spectral data acquired on different instruments and/or computers can be compared to one another.

COMPRO has been upgraded 5 times and the present version is 5.4. COMPRO runs on Windows and can be downloaded from the home page of Surface Analysis Society of Japan(SASJ), for which the address is "sekimori.nrim.go.jp".

2. File format conversion

The VAMAS community decided to use the VAMAS Standard Data Transfer Format [3] as a common data format. This format is now approved as ISO-14976. However, this data format defines mainly the measurement conditions such as sample positioning, analyzer alignment and so on. To share spectral data, the data format should also carry information on the specimen, analyzer calibration, and data processing. To attach this information to the spectral data format, an information format has been proposed as ISO-DIS-14975 [4]. The information format is made up of blocks; these are the specimen information block, the calibration information block and the data processing information block. Each block has its own identifier, and so a programmer can easily prepare reading software. The Information format can be inserted into the

VAMAS/ISO format and is completely compatible with it.

COMPRO can convert an original data format to the VAMAS/ISO format, if the original file is written in ASCII(text) code. COMPRO automatically searches the count data array of the original data format, and displays count data on the screen. The user will then enter energy scales and other necessary information manually. COMPRO also provides the database with default measurement conditions for the major commercial instruments. By using this database, one can easily insert the required items by the VAMAS/ISO format.

If the file structure is converted to the VAMAS/ISO format, one can display the information in a spectrum with COMPRO. Figure 1 shows specimen, calibration, and data processing information blocks displayed by COMPRO. One can enter or modify information on this screen.

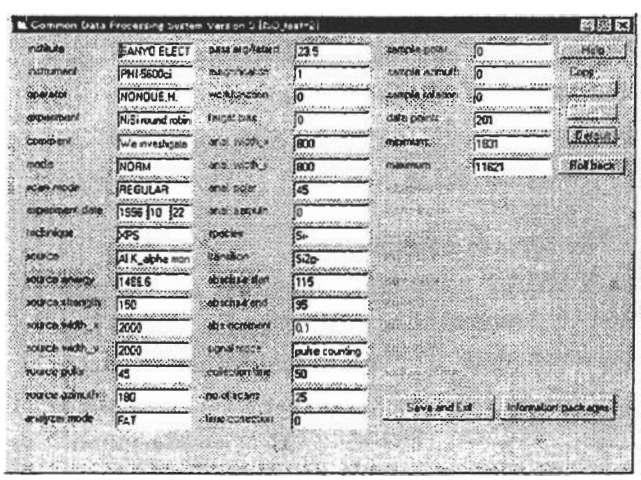

Fig.1 Information on spectrum displayed on COMPRO

3. Spectrum display

Once spectrum data is converted to the VAMAS/ISO format, a spectrum can be displayed on the computer screen, then zoomed, deconvoluted, smoothed, differentiated, background subtracted, or peak fitted. COMPRO has a database for peak energy values of elements. By moving a cursor on the screen, one can identify the peak as shown in Fig.2. COMPRO can covert not only spectral data but also depth profile data according to the VAMAS/ISO format.

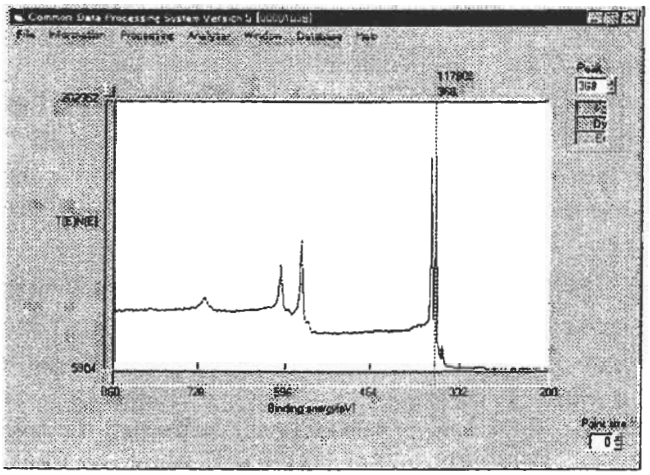

Fig.2 Peak assignment using the database in COMPRO

4. Energy scale calibration

The energy scale calibration is done by referring to the standard peak data of Ag, Au, and Cu proposed by Seah, Smith, and Anthony for AES [5] and Anthony and Seah for XPS[6]. When one inputs peak energies of more than three transitions obtained by one's spectrometer, the energy dependence of deviations from the reference peak energies is plotted and can be recorded in a form of an offset function, where an offset function is given by the following equation.

$$E_{(calibrated)} = E_{(observed)} + \text{offset function}$$

where

$$\text{Offset function} = X^*E + Y$$

(E: energy, X and Y: constant)

The usefulness of the offset function has been already reported [7]. Therefore, it is important to attach observed values for Ag, Au and Cu peaks to share the spectral data. These observed values can be stored in the Information formats of the spectral data, if one uses the ISO Information formats (ISO-DIS-14975). COMPRO provides a tool to add observed values for energy scale calibration to spectral data. When the spectral data carries the necessary information on energy scale calibration, COMPRO finds information on calibration, and displays the calibrated spectrum. This procedure is done by clicking a menus of COMPRO.

5. Intensity scale calibration

The energy dependence of the intensity scale is called the spectrometer function and is defined

as follows:

$I(E) = I_s * Q(E) * n(E)$

where I_s is the primary beam flux, $Q(E)$ is the spectrometer function, and $n(E)$ is the true distribution of emitted electrons from the sample [8].

The intensity scale evaluation is done by referring to standard spectra. If one divides one's spectrum with the standard spectrum, one can obtain the 'relative' spectrometer function which is called 'calibration' function in COMPRO. COMPRO recommends use of the Au or the Cu spectrum for intensity scale calibration. COMPRO provides standard Au and Cu in the spectra database. Therefore, if one uses COMPRO, intensity scale of the reported spectrum is normalized to the standard spectrum in COMPRO.

The 'standard' spectra are defined as spectra which will be used to calibrate the intensity and energy scales of one's spectrometer [8,9]. Several 'standard' spectra for calibration have been reported [10,11]. In COMPRO, the AES spectra taken by Professor K.Goto of Nagoya Institute of Technology, are included as the standard spectra, because these spectra are available as digital data. The XPS 'standard' spectra in COMPRO were taken on a double-pass CMA which has an E_k^{-1} dependency [12].

COMPRO provides a calculation routine for the calibration function as shown in Fig.3. Figure 3 shows the result of getting a 'calibration' function for AES using the Cu spectrum. By changing parameters based on the secondary electron emission coefficient of multiplier, one finds a best fitting set of parameters to calculate the 'calibration' function [13]. At present, the calibration function calculated based on parameters of a multiplier is stored. However, the function fitted with a simple polynomial will also be available in future.

Therefore, to attach information on the intensity scale to the spectral data, one should attach an Au or Cu spectrum to the reported spectral data. When one uses COMPRO, this attachment procedure is easily done, and the file structure according to ISO-DIS-14975 is automatically created. When the spectral data carries a calibration file, COMPRO detects the information on calibration, and informs the user to calculate the calibration function for the intensity scale by clicking a COMPRO menu.

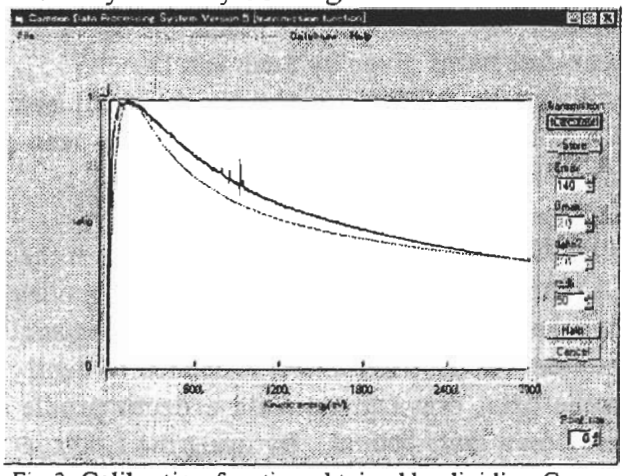

Fig.3 Calibration function obtained by dividing Cu measured spectrum by a standard spectrum

6. Data processing

One can process spectral data by clicking the menu of COMPRO. COMPRO can calibrate a spectrum if it carries a calibration data file as explained in section 4 and 5.

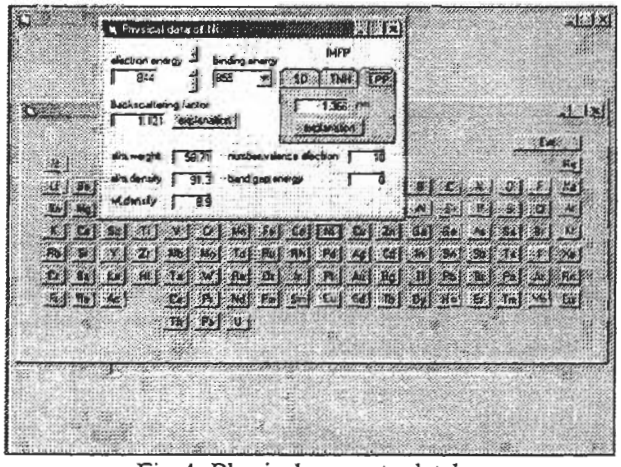

Fig.4 Physical property database

7. Databases

COMPRO has a reference spectral database created by the voluntary work of SASJ members and a physical properties database; these are available, if one downloads and installs "BankData.exe" file from the Internet. From the COMPRO menu, one can get reference AES or XPS spectra by clicking on an elemental table, and atomic information such as atomic density and weight density.

COMPRO also has a database of electronic information such as number of valence electrons and band gap energy. A list of binding energies is also available. The backscattering correction factors given by Shimizu and Ichimura [14] and the inelastic mean-free paths given by Seah and Dench [15], by Tokutaka, Nishimori, and Hayashi [16] and by Tanuma, Powell, and Penn [17] can be seen.

8. Depth profile analysis

COMPRO can analyze depth profile data in the VAMAS/ISO format by the MRI model proposed by Hofmann [18] or by a Logistic function. When MRI model is applied to depth profile data, one can simulate a depth profile based on a layer model. By using the Logistic function routine, one can get the depth resolution defined by the 16%-84% method as shown in Fig.5

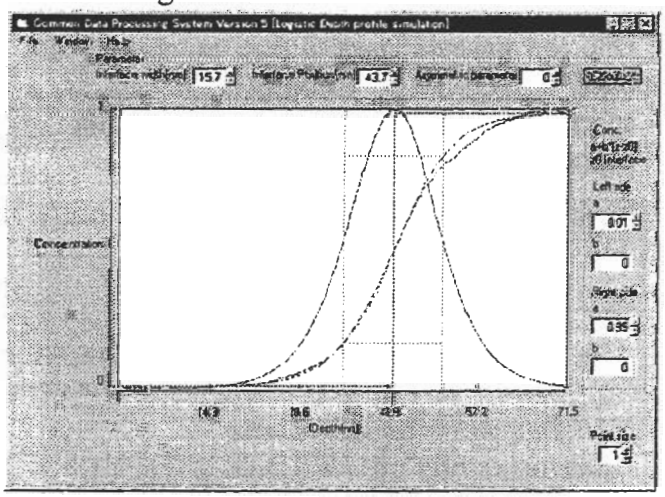

Fig.5 Depth profile resolution function obtained by using Logistic function

9. Summary

In this paper, an outline of COMPRO Version 5 is introduced. The main objectives of COMPRO are to provide a tool for sharing spectral data and a common bed for data processing procedures proposed by scientists. By using COMPRO, one can convert the format of spectral data and depth profile data to the VAMAS/ISO format, and attach calibration information of the energy and intensity scales to the spectral data. At present, COMPRO has data processing algorithms such as zooming, deconvolution, differentiation, smoothing, background subtraction, peak fitting, and so on. COMPRO welcomes data processing algorithms proposed by users.

Acknowledgment

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