

Common Data Processing System Version 7

Kazuhiro YOSHIHARA

National Institute for Materials Science, 1-2-1, Sengen Tsukuba 305-0047, Japan

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We have been constructing the spectral data processing system under VAMAS (Versailles Project on Advanced Materials and Standards) umbrella since 1989. This system is called Common Data Processing System (COMPRO). COMPRO is designed to be a program to convert an original spectral data file structure to ISO14975 and 14976 formats, to assess the data processing procedures proposed by scientists, to calibrate energy and intensity scales, to check a spectrum, and to build both spectra and correction factor database. In this system, the spectral data acquired on different instruments and/or computers can be compared to one another. COMPRO has been upgraded many times, and the latest one is Version 7, which runs on Windows95/98/NT/Me/XP. Major updated points of Version 7 are (1) manual format conversion routine, (2) Prof. Goto's AES absolute spectra database, (3) Thickogram routine, (4) ISO energy scale calibration, (4) Information on ISO activities.

1. Introduction

About 30 years have passed since commercial AES and XPS apparatuses appeared. Since that time, a number of spectral data for surfaces were 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 spectral database, we have to establish the system to share spectral data taken on different machines.

Since 1989, we have been constructing the spectral data processing system under VAMAS (Versailles Project on Advanced Materials and Standards) umbrella [1,2]. This system is called Common Data Processing System (COMPRO). COMPRO is designed to be a program to convert an original spectral data file structure to common one [3], to assess the data processing

procedures proposed by scientists, to calibrate energy and intensity scales, to check a spectrum, to check the feasibility of the data processing algorithms proposed by scientists, and to build both spectra and correction factor database. In this system, the spectral data acquired on different instruments and/or computers can be compared to one another.

COMPRO has been upgraded 7 times and the present version is 7.1. The objective of the paper is to introduce the latest version of COMPRO. COMPRO (present version is 7.1) runs on Windows and can be downloaded from the home page of Surface Analysis Society of Japan [<http://www.sasj.gr.jp>].

2. File format conversion

VAMAS community decided to use 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 measurement conditions such as sample positioning, analyzer alignment and so on. To share spectral data, data format should also carry the information on specimen, analyzer calibration, and data processing. To

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attach this information to the spectral data format, ISO 14975 is determined [4]. Information formats are made of blocks, which are specimen information block, calibration information block and data

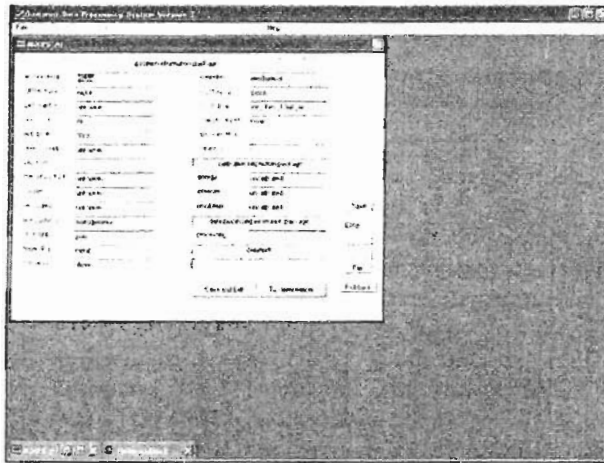


Fig.1 Information on spectrum displayed on COMPRO

processing information block. Each block has own identifier, so a programmer can easily prepare reading software. The Information formats can be inserted into ISO 14976 format and is completely compatible with it.

COMPRO can convert an original data format to ISO format, if the original file is written in text code. COMPRO principally converts the format into ISO 14976 automatically, but it sometimes cannot change. In this case, COMPRO provides the manual conversion routine using a flexible grid sheet. By this routine, COMPRO can convert any text data file to ISO 14976 format. COMPRO also provides the database for default measurements conditions of major commercial instruments. By using this database, one can easily insert the requested items by ISO 14976. COMPRO can convert not only spectral data but also depth profile data to ISO format.

Once the file structure is converted to ISO format, one can display the spectrum and the information on that spectrum. Figure 1 shows specimen, calibration, and

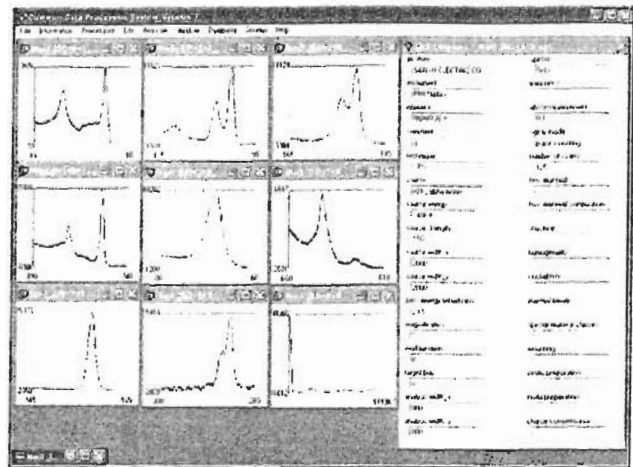


Fig.2 Display of multi regions

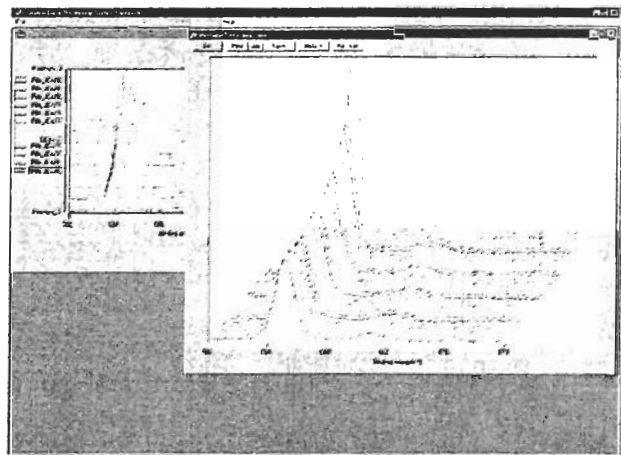


Fig.3 Bird's eye view of a series of spectra

data processing information blocks (according to ISO 14975) displayed by COMPRO. One can enter or modify information on this screen.

3. Spectrum display

Once spectrum data is converted to ISO format, a spectrum can be displayed on a computer screen, then zoomed, deconvoluted, smoothed, differentiated, background subtracted, or peak fitted. COMPRO adopts MDI (multi document interface) system, so, multi regions of spectrum are displayed simultaneously as shown in Fig.2. To analyze the shape change of spectra by such as sputtering or radiation damage, COMPRO can display the series of spectra by bird's eye view as shown in Fig.3

4. Analyzer 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]. Recently, ISO 15472 reported the energy scale calibration for XPS. These calibration procedures are basically based on the use of offset function given by the following equation.

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

where offset function = $X * E + Y$
 (E : energy, X and Y : constant)

The usefulness of the offset function has been already reported[7]. COMPRO provides these calibration processes.

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 the standard spectra. If one divides one's spectrum with the standard spectra, one can obtain the 'relative' spectrometer function which is called 'calibration' function in COMPRO. COMPRO recommends using Au or Cu spectrum for intensity scale calibration. COMPRO provides the Au and Cu 'standard' spectra database[9,10]. Therefore, if one uses COMPRO, intensity scale of the reported spectrum is normalized to the standard spectrum in COMPRO.

5. Data processing

At present, COMPRO has data processing algorithms such as zooming, deconvolution, differentiation, smoothing, background subtraction, peak fitting, and so on. COMPRO has a database for peak energy values of elements. Figure 4 shows the result of Tougaard background subtraction by COMPRO. To assist the document presentation of users, the

displayed screen before/after data processing can be stored as a bit map image. By using this database, one can identify the peak automatically or manually. To quantify the surface concentration, COMPRO provides databases for relative sensitivity factors.

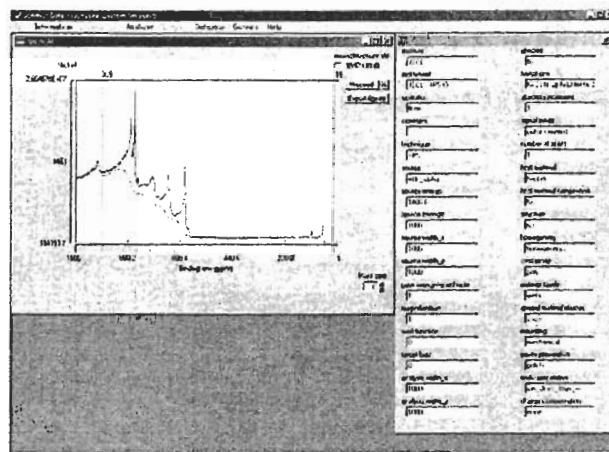


Fig.4 Result of Tougaard background subtraction

6. Databases

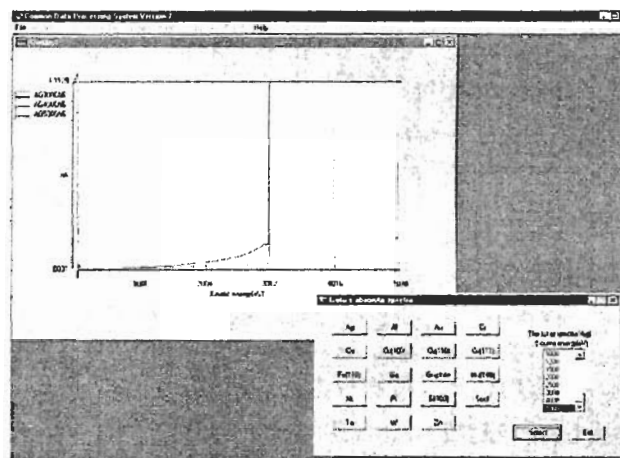


Fig.5 The Ag absolute spectra measured by Prof. Goto

COMPRO has reference spectral database created by the voluntary work of SASJ members and physical properties database. From the menu of COMPRO, one can get reference AES or XPS spectra by clicking elemental table, and atomic information such as atomic density and weight density. COMPRO also has a database for AES absolute spectra

measured by Prof. Goto. The intensity scale of AES absolute spectra is [nA]. The Ag absolute spectra are shown in Fig.5 by changing the source energy of primary electron beam.

COMPRO has also the database of electronic information such as number of valence electrons and band gap energy. The list of the binding energies is also

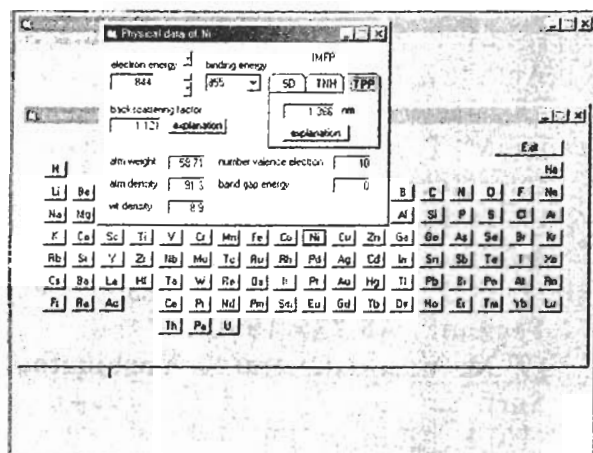


Fig.6 Physical property database

available. The backscattering correction factors given by Shimizu and Ichimura[11] and inelastic mean-free paths given by Seah and Dench[12], by Tokutaka, Nishimori, and Hayashi[13] and by Tanuma, Powell, and Penn[14] can be seen.

7. Depth profile analysis

COMPRO can analyze depth profile data with ISO format by MRI model proposed by Hofmann[15] or Logistic function. When MRI model is applied to depth profile data, one can get the simulated layer model, if a data structure of spectrum is ISO format. The screen for MRI process is shown in Fig.7. By using Logistic function routine, one can get the depth resolution defined by 16%-84% method.

Recently, Cumpson proposed the simple routine for calculating the thickness of thin film[16]. This routine is called *Thickogram*, and is incorporated in COMPRO as shown in Fig.8.

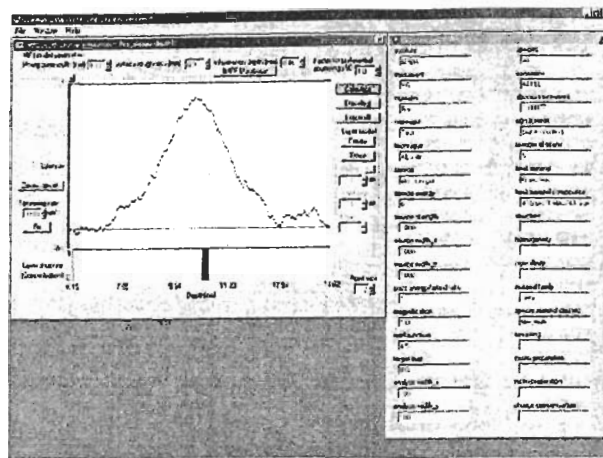


Fig.7 Depth profile analysis by MRI model

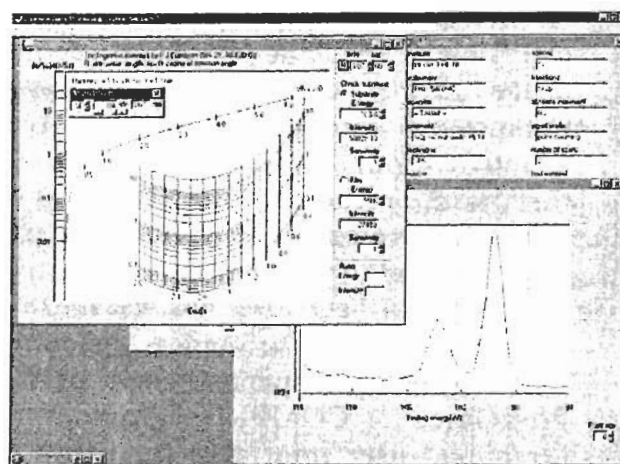


Fig.8 Calculation of the thickness of thin film by Thickogram

8. ISO information

By clicking the help menu, the recent information on ISO TC201 activities is displayed as shown in Fig.9. By this help menu, user can get the guideline of ISO regulations.

9. Summary

In this paper, the outline of COMPRO Version 7 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 ISO format, and attach calibration information of energy and intensity scales to a spectral data.



Fig.9 Help menu for ISO information

At present, COMPRO has data processing algorithms such as zooming, deconvolution, differentiation, smoothing, background subtraction, peak fitting, quantification, qualification, film thickness measurement and so on. COMPRO welcomes to include other data processing algorithms proposed by users.

COMPRO also has databases for standard spectra, reference spectra and AES absolute spectra measured by Prof.Goto. COMPRO provides GUI (graphical user interface) for using these databases.

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