

## The Development of the Common Data Processing System

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This paper introduces the history of the development of COMPRO (Common Data Processing System). We have been constructing the spectral data processing system named COMPRO under VAMAS (Versailles Project on Advanced Materials and Standards) umbrella since 1989. Since the initial stage of the project, Dr. Sekine was a main contributor to the development of 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. Dr. Sekine pointed out the importance of the spectral databases to create the common world of surface analysis. By his suggestions, COMPRO decided to include both "reference" and "standard" spectra databases. 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.

### INTRODUCTION

VAMAS Project (Versailles Project on Advanced Materials and Standards) was set up at the Economic Summit of Versailles in June 1982. A number of technical working parties have been organized, one of which is TWA 2 (Surface Chemical Analysis) chaired by Dr. M. P. Seah (at present, Dr. C. Powell). In 1987, Japan decided to participate in the VAMAS-TWA 2 activity, and organized the Japanese committee, the chairman of which was Prof. R. Shimizu. Since that time, Dr. Sekine had been an active member of the committee and carried out many useful projects to improve the reliability of surface analysis. Under the VAMAS umbrella, we started the project on the estimation of quantitative reliability of AES by using Co-Ni alloys (VAMAS Project No.20). To execute this project, we had to process the spectral data taken on different machines. Therefore, we had to determine the common data structure of spectral data to process the spectral data in computers.

In July 1989, Dr. Sekine surveyed the VAMAS-SCA Standard Data Transfer Format[1], and proposed the partially encoded version of the VAMAS-SCA Standard Data

Transfer Format. A memory system of a computer was very poor at that time, and we had to invent the partially encoded version of the format to save memories of computers. After the partially encoded version was determined, we announced the construction of the software to convert the original data format taken on different machines to the partially encoded version of VAMAS - SCA Standard Data Transfer Format.

### COMMON DATA PROCESSING SYSTEM VERSION 2

In 1990, the projects started to construct software in Quick Basic for IBM PC or NEC PC with MS-DOS to translate spectral data acquired on different machines to the VAMAS - SCA Standard Data Transfer Format and to construct software to manipulate AES and XPS spectra in a standard manner (VAMAS Project No.30). The software was called Common Data Processing System, and Version 2.0 was released in April 1991[2]. The opening screen of Version 2.0 is shown in Fig. 1. This version could convert the data formats of spectra taken on instruments of major manufacturers to the standard one. To construct this soft-

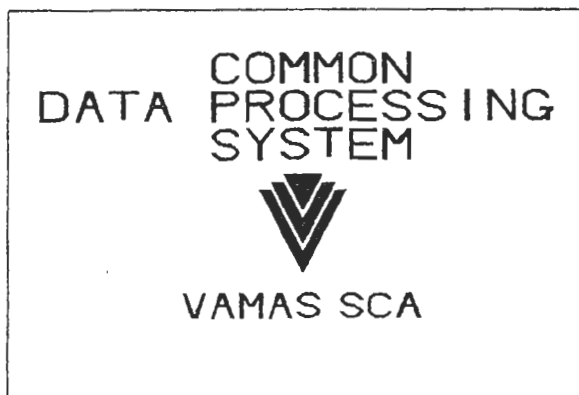


Fig. 1. The opening screen of Version 2.0.

ware, major manufacturers opened their own data format structures to our committee by the intensive help of Dr. Sekine. By this process, we could accumulate many spectral data with the common data file structure, and the committee members became aware of the importance of spectral database to improve the reliability of surface chemical analysis. Therefore, in this version, spectral database was incorporated by the committee members.

In December 1991, International Symposium on Pre-standard Research for Advanced Materials (ISPRAM 91) was held in Tokyo. In this symposium, Dr. Sekine lectured on spectral database and pointed out the importance of network system to share the spectral data[3]. Unfortunately, at that time, computers could only be connected by modems of slow transmission rate, and it took very long time to transfer one spectrum. So, his idea could not be realized at that time, but nobody could foresight that computers in the world could be connected by the high speed Internet. His idea had been realized by the project on the construction of Internet database which started in 1994 by the support of Science and Technology Agency, Japan.

### COMMON DATA PROCESSING SYSTEM VERSION 3

In 1994, new operation system for computer called Windows 3.1 became popular, and MS-DOS system became outdated. Version 2 could not run on Windows as it was. Therefore, the Common Data Processing System had been translated into the software in Visual Basic with Windows and some important reforms have been made[4, 5]. The screen for the format conversion routine of Version 3.1 is shown in Fig. 2. The display style of Common Data Processing System has been almost fixed since this ver-

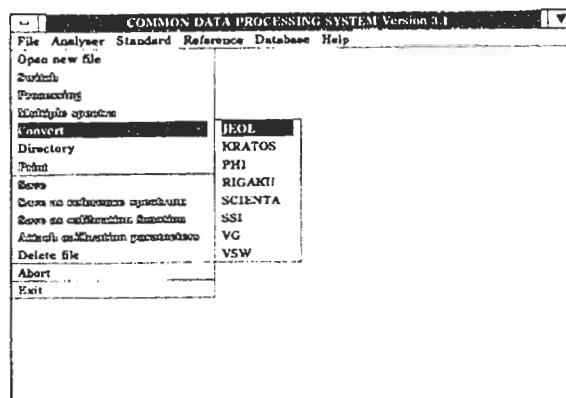


Fig. 2. The screen for the format conversion routine of Version 3.1.

sion, and the software called COMPRO.

### PRESENT VERSION OF COMPRO

COMPRO has been upgraded 7 times. Version 5 was introduced in journals[6,7]. The present version is 7.1[8]. From version 4, COMPRO can be downloaded from the home page of Surface Analysis Society of Japan [http://www.sasj.gr.jp]. The opening screen of Version 7.1 is shown in Fig. 3.

### File format conversion

VAMAS Standard Data Transfer 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 attach this information to the spectral data format, ISO 14975 is determined[9]. Information formats are made of blocks, which are specimen information block, calibration information block and data processing information block. Each

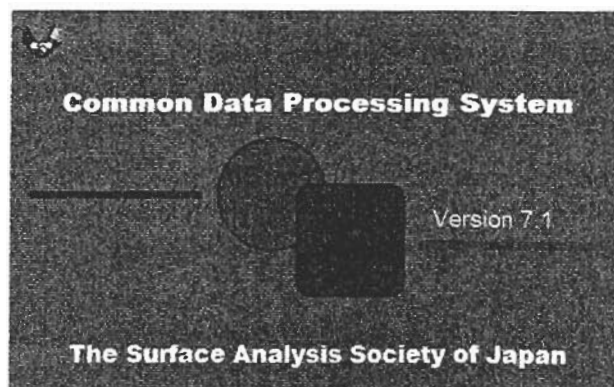


Fig. 3. The opening screen of Version 7.1.

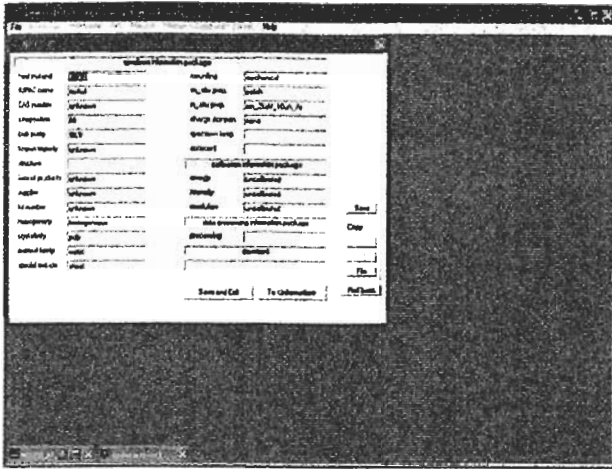


Fig. 4 Information on spectrum displayed on COMPRO.

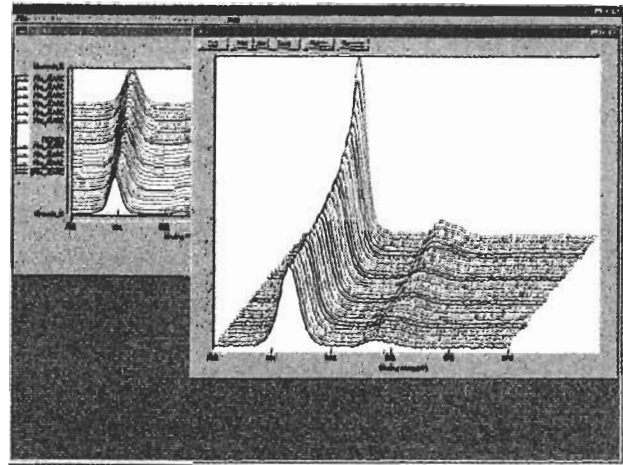


Fig. 6 Bird's eye view of a series of spectra.

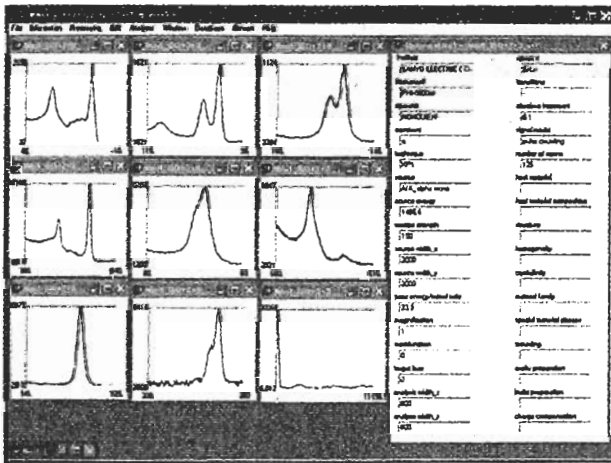


Fig. 5. Display of multi regions.

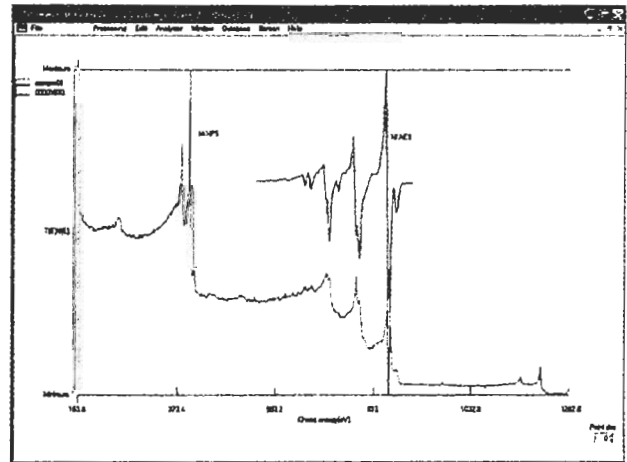


Fig. 7. XPS and AES Ni spectra displayed on the same screen.

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. A computer has improved the memory system, and it is not necessary to use the partially encoded version of VAMAS-SCA Standard Data Transfer Format any more. 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 4 shows specimen, calibration, and data processing information blocks (according to ISO 14975) displayed by COMPRO. One can enter or modify information on this screen.

### 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. 5. 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. 6

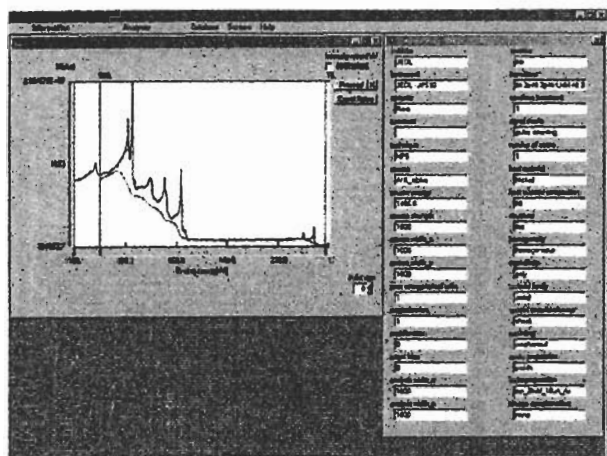


Fig. 8 Result of Tougaard background subtraction

One of the initial objectives of COMPRO project was to display the different kind of spectra on the same screen of a computer as shown in Fig. 7.

#### 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[10] and Anthony and Seah for XPS[11]. Recently, ISO 15472 reported the energy scale calibration for XPS. COMPRO supports the energy scale calibration procedure by using 'offset function'[12].

The intensity scale evaluation is done by referring to the standard spectra in COMPRO. 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[13,14]. Therefore, if one uses COMPRO, intensity scale of the reported spectrum is normalized to the standard spectrum in COMPRO.

#### Data processing

One of the main objectives of COMPRO is to produce the common bed to check the feasibility of the data processing procedure proposed by scientists. At present, COMPRO has data processing algorithms such as zooming, deconvolution, differentiation, smoothing, background subtraction, peak fitting, and so on. Figure 8 shows the result of Tougaard background subtraction by COMPRO. To assist the document presentation of users, the dis-

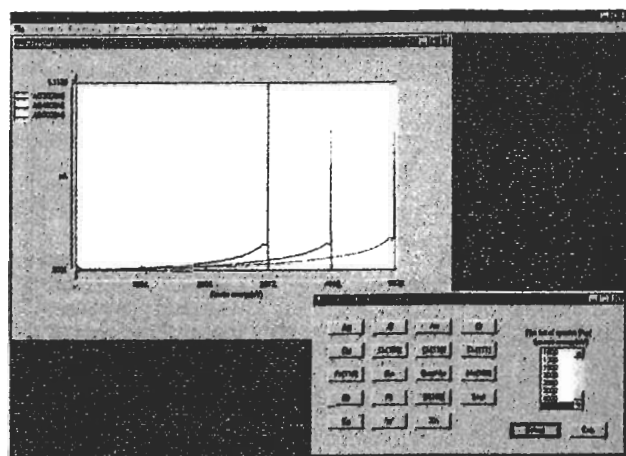


Fig. 9 The Ag absolute spectra measured by Prof. Goto

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

#### Databases

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. 9 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 available. The backscattering correction factors given by Shimizu and Ichimura[15] and inelastic mean-free paths given by Seah and Dench[16], by Tokutaka, Nishimori, and Hayashi[17] and by Tanuma, Powell, and Penn[18] can be seen.

#### Depth profile analysis

COMPRO can analyze depth profile data with ISO format by MRI model proposed by Hofmann[19] or Logistic function. When MRI model is applied to depth profile data, one can get the simulated layer model, if a data struc-

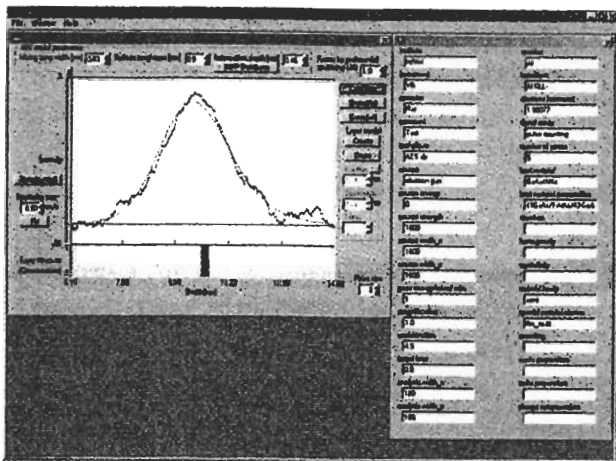


Fig. 10 Depth profile analysis by MRI model.

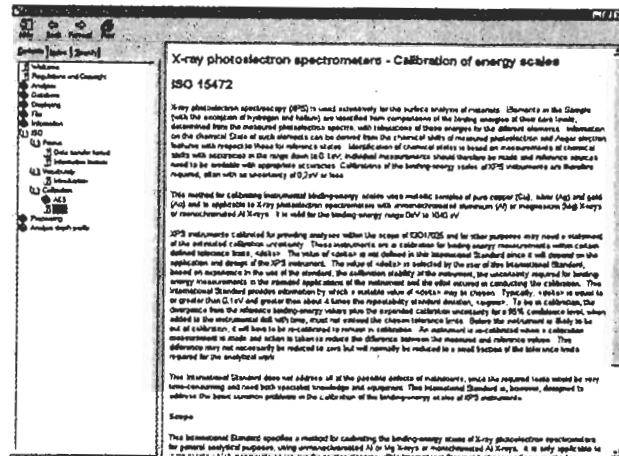


Fig. 12 Help menu for ISO information.

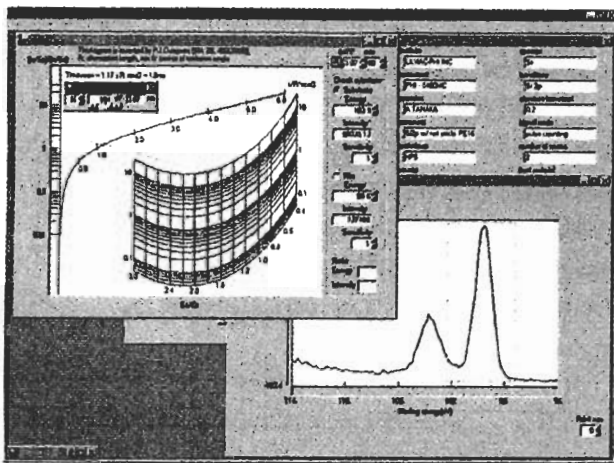


Fig. 11 Calculation of the thickness of thin film by Thickogram.

ture of spectrum is ISO format. The screen for MRI process is shown in Fig. 10. 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[20]. This routine is called *Thickogram*, and is incorporated in COMPRO as shown in Fig. 11.

**ISO information**

By clicking the help menu, the recent information on ISO TC201 activities is displayed as shown in Fig.12. By this help menu, user can get the guideline of ISO regulations.

**SUMMARY**

In this paper, the history of COMPRO 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. This idea was created in the discussion at the committee meetings for VAMAS activity, and one of the leaders in the discussion was Dr. Sekine. Without his contribution, we could not have carried out the COMPRO project.

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. The present version of COMPRO is version 7.1. 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.

**ACKNOWLEDGEMENT**

Dr. Sekine was the inventor of the common world for surface analysis. By his guide, author has been able to carry out the project to develop COMPRO. Author also expresses his sincere thanks to the members of Surface Analysis Society of Japan for their voluntary work to check the feasibility and fix bug problems of COMPRO.

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