Construction of the Surface Analysis Network Database

Kazuhiro Yoshihara and Michiko Yoshitake
National Institute for Metals
1−2−1, Sengen, Tsukuba, 305 Japan

In 1994 the Science and Technology Agency (STA) of Japanese Government launched a project to interconnect networks under various ministries and agencies. The project is called Inter−Ministry Computer Network System (IMNet). Every site joining to IMNet would have a connection with 600M bps to one of NOCs (Network Operation Centers) located in Tsukuba − Tokyo − Osaka. As a site of IMNet we are implementing a network−oriented database for surface chemical analysis such as AES and XPS spectra. A workstation has been installed to collect the spectral data for different analysis machines via computer networks and modem lines. In future we hope all computers of the surface analysis machines can be connected to the system so that every surface analyst worldwide can share the spectral data and the common data processing software to identify the surface chemistry of new materials.

(*Received 13 October 1995*)

1.Introduction

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. The Common Data Processing System 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 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. The Common Data Processing System is not commercially produced.

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2. Features of the surface analysis database

NIST has published a database for XPS peak positions. AVS is publishing *Surface Science Spectra*. Manufacturers have their own spectral databases and distributed to their customers. Usually, the objective of these databases is to provide users with spectral data of clean surfaces of pure materials. However, the concept of this database is that "If we store the all spectral data of all surfaces taken on all machines, we can characterize any surfaces and calibrate any analyzers without difficulty". This concept is different from those of other existing databases, and we consider this database should be open to public.

A workstation was installed in National Research Institute for Metals to collect the spectral data with VAMAS format[3] from different analysis machines via computer networks and modem lines. Collected spectra are stored in the database. The surface analysis database can be accessed via "WWW InterNet". If a personal computer is connected to InterNet, one can access the home page of the Surface Analysis Society of Japan(SASJ), which address is "sekimori. nrim. go. jp". The connection image is shown in Fig.1. SASJ is responsible to provide the spectral data, and controls its quality. When the home page of SASJ is opened, one can select the database menu and retrieve a spectrum from the selection menu. The retrieved spectrum will be displayed on a screen as a "GIF" image. If the personal computer has already the Common Data Processing System in its memory, a retrieved spectrum can be downloaded by using the programs in it. The member of SASJ will be provided with the Common Data Processing System.

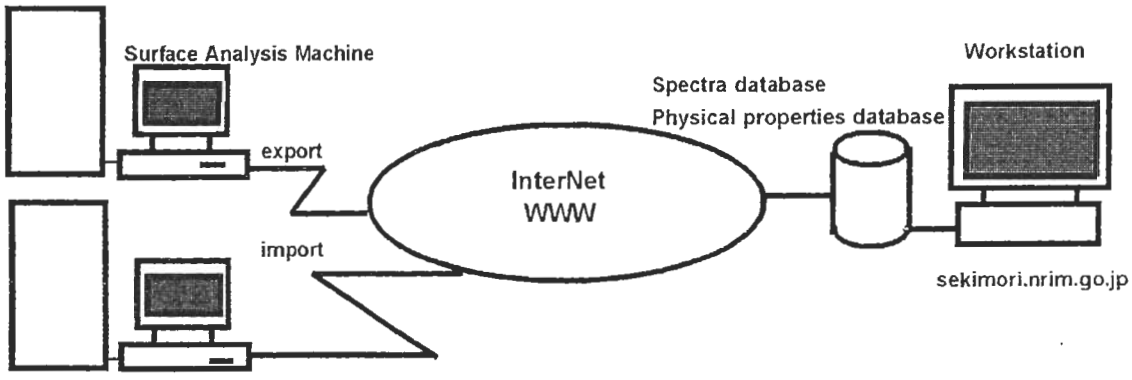

Fig.1 Connecting image of the network-oriented surface analysis database

3. Spectral database and its significance

A useful spectral database for surface analysis should contain both "standard" spectra and "reference" spectra. The "standard" spectra will be used to calibrate the intensity and energy scales of one's spectrometer[4,5]. The several "standard" spectra for calibration have been reported[6,7]. However, in this database, the AES spectra taken on the mechanically well-defined analyzer, which had been developed by Professor K.Goto of Nagoya Institute of Technology, are included as the standard spectra. This analyzer has a specially designed CMA and is operated in FRR mode. The details of the analyzer are described elsewhere[6]. The XPS spectra in the "standard" spectra database were taken on a double-pass CMA. The double-pass CMA has both FRR and FAT modes. By this dual mode, it was determined that the FAT mode of the double-pass CMA, which retards electrons by two spherical meshes before CMA, has Ek^{-1} dependency[8]. The Surface Analysis Society of Japan rates these "standard spectra" at "class s". So, one can retrieve a standard spectrum from database by using the keyword of "class s".

The "reference" spectra are collected through the voluntary work of the members of SASJ using certified materials. The quality of spectra is checked by the committee of SASJ. The committee checks the calibration procedures for energy and intensity scales of a supplier's analyzer, and rate a spectrum sent from a supplier. The reference spectra will be used to identify the surface chemistry of new materials by comparing it with an obtained spectrum.

4. Physical properties database

The objective of the surface analysis database is not only to construct a spectra database but also to create a physical properties database. The Common Data Processing System has already physical properties database. From the menu of the Common Data Processing System, one can get atomic information such as atomic density and weight density, and electronic information such as number of valence electrons and band gap energy are listed. The list of the binding energies also appears. The backscattering correction factors given by Shimizu and Ichimura[9] and inelastic mean-free paths given by Seah and Dench[10], by Tokutaka, Nishimori, and Hayashi[11] and by Tanuma, Powell, and Penn[11] can be seen. We intend to incorporate this type of physical properties database into the network-oriented surface analysis database.

5. The retrieval procedure for the spectra database

The spectra database has an index[13]. When a spectra is registered in the database, the index is renewed. The necessary information for the registration must be attached with the spectrum sent by a supplier. The spectral data transfer format is being discussed in ISO/TC201 committee. However, the spectral data of VAMAS format[3] is acceptable until the final format is determined by ISO committee. The content of the index is shown in **Table 1**. The structure of index is still under discussion. Therefore, at present, encoded version of the index has been created in the workstation. The index of the encoded version is composed of the underlined items shown in Table 1. The index is created using "Oracle" database engine, and easily retrieved by SQL language. However, it is impossible for a person who does not know SQL language to retrieve a spectrum. Therefore, the spectra database provides a user with an graphical user interface(GUI). **Figure 2** shows GUI for the retrieval procedure for the database. When a user inputs or selects searching condistions for spectra from the computer screen, the list of the

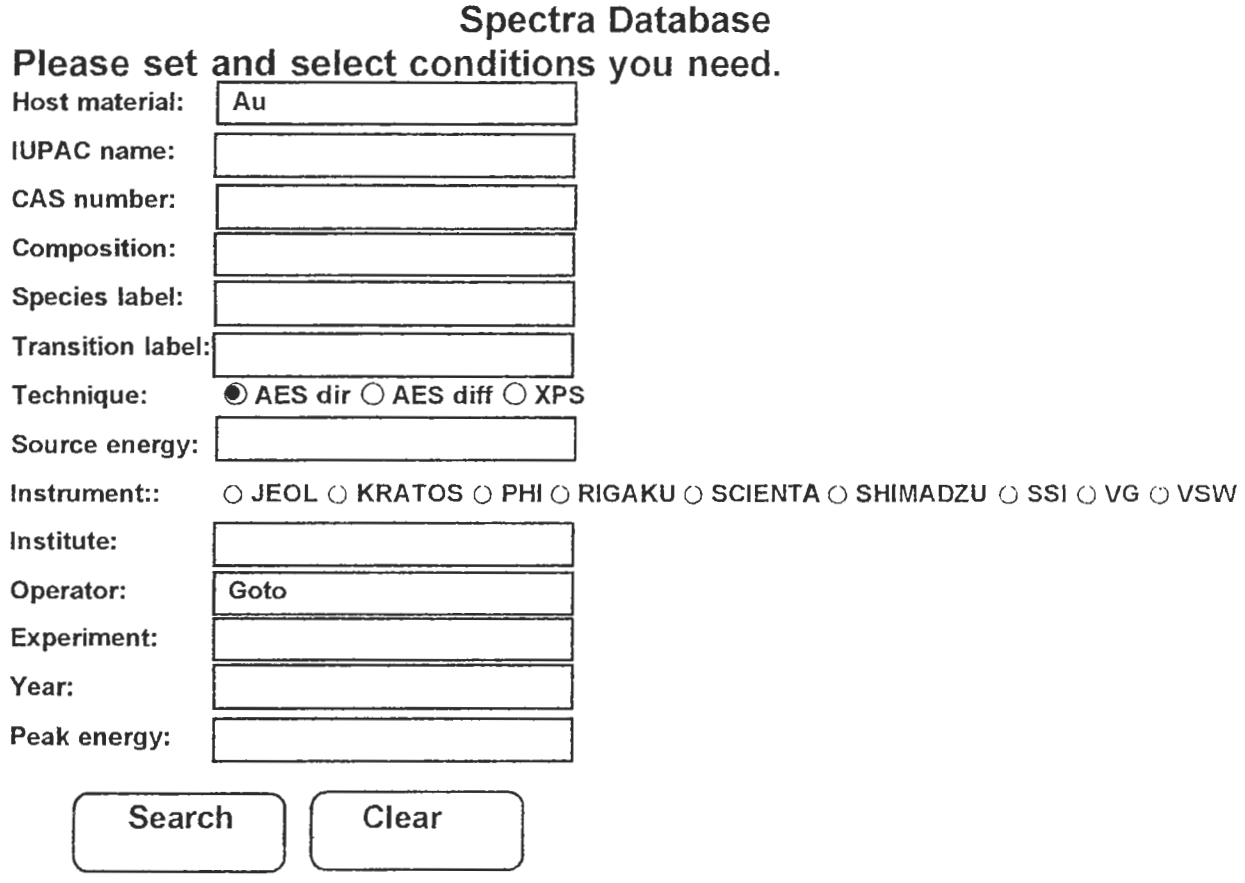

Figure 2 The retrieval image of spectra database

spectra which corresponds to the selection is shown. When a user selects one of the spectra in the list, the retrieved spectrum is shown onthe screen. If a user has already installed the Common Data Processing System in the personal computer, the retrieved spectrum can be stored in the computer and processed or compared with other spectral data. In the near future, we intend to incorporate the searching software using a spectral shape.

6. Hardware configurations

To access to the surface analysis database, users should connect their computers to InterNet. If user's organization has not connected to InterNet, an user's computer is recommended to connect InterNet personally. Nowadays, there are many companies which provide with connecting service to InterNet. Users should contact one of those providers, and purchase a recommended modem. To use InterNet, users also install the browser 'netscape' to its own computer. 'netscape' is available commercially.

7. Summary

In this paper, the basic concept of the database and the retrieval system for spectral data via computer network are introduced. In future we hope all computers of the surface analysis machines can be connected to the system so that every surface analyst worldwide can share the spectral data and the common data processing software to identify the surface chemistry of new materials.

Acknowledgment

Authors express their sincere thanks to the members of Surface Analysis Society of Japan for their voluntary work. Mr.S.Yamamoto, Mr.H. Kurokawa, and Mr.R.Kawasaki of NTT Corporation are also acknowledged for creating a retrieval software in WWW InterNet.

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Comments & Replies

Referees

A: Shingo Ichimura(ETL)
B: Tetsu Sekine(JEOL Ltd.)

A-1: Construction of database relating surface analysis has been proposed by several research organizations, It is recommended that the authors refer them and make clear the specific feature of the Surface Analysis Database.

Author-A1: As the referee pointed out, a number of databases has been published already. I described the present status in the chapter 2.

A-2: As the Surface Analysis Database is accessible through InterNet, it is obvious that anyone can refer the database. Is there any difference for the usage of the network database between member and non-member of the SASJ ?

Author-A2: Anyone can access to the database. However, the member of SASJ can download the spectral data from the database. This was indicated in chapter 2.

B-1: Please check the year when the development of the project on the Common Data Processing System started.

Author-B1: The project started at 1989, and Version 2 was distributed in 1990. It was indicated in Chapter 1.

B-2: Title of chapter 2 should be changed to "Spectral database and its significance".

Author-B2: I changed the title as indicated.

B-3: What kind of tools do we need to access to the surface analysis database in terms of hardware and software.

Author-B3: I created a new chapter entitled "Hardware Configurations", and wrote about the necessary tools.

B-4: If we got it, do we get a reasonable response for the communication with it.

Author-B4: The access time depends on the hardware configuration to retrieve the spectral data. Usual access time is reasonable, even if one uses modem line.

Table 1 Index for the spectra database

Item	Meaning	Example
FileId	File Identifier	00000104
InstId	Institution Identifier	NRIM
ModlId	Instrument Model Identifier	PHI-660
OprtId	Operator Identifier	Yoshihara
ExprId	Experiment Identifier	quantify
Commnt	Comment	Round robin
ExpMod	Experiment Mode	NORM
NumRgn	Number of Spectral Regions	2 (After registration, NPL file -> 1)
NumBlk	Number of Blocks	3 (〃 , NPL file -> 1)
BlckId	Block Identifier	4th block id (〃 , NPL file ->1st block)
SmplId	Sample Identifier	1st sample id
YearIF	Year in full	1991
MonthY	Month	4
DayMnt	Day of Month	12
DHProc	Data Handling Procedure	differentiated
ErgScl	Energy Scale Calibration Procedure	C ("C" means "calbrated by the Cu***")
IntScl	Intensity Scale CalibrationProcedure	A: Cu spectrum(Num:********) is attached
ResScl	Energy Resolution CalibrationProcere	none
HostMt	Host Material (common name)	stainless steel
IUPACn	IUPAC Chemical Name	unknown
CASNum	Chemical Abstracts Registry Number	unknown
HostCm	Host Material Composition	Fe 74 Cr 18 Ni 8
BlkPrt	Bulk Purity	99.9
Strctr	Structure	fcc
FormPr	Form of Products	Roof
Crystn	Crystallinity	P
MatFam	Material Family	M
MatCls	Special Material Classes	C
ExPrep	Ex situ Preparation	polish
InPrep	In situ Preparation	ion sputtering
SmpTmp	Specimen Temperature	298
ChgCnt	Charge Control Conditions	none
ElmExt	Elements Existing on the Surface	Fe-Co-Ni
SmpInf	Specimen Information	supplied by NRIM
SpcInf	Spectrum Information	AF0045RT 4th of 6 blocks (original name and blocks)
SpcGrp	Spectrum Group	00000101-00000106(Group spectra)
SpcRnk	Spectrum Ranking	R
Techng	Technique	AES dir
AnlSrc	Analysis Source Label	electron gun
AnlErg	AnalysisSource Characteristic Energy	5000
TakOff	Analyser Axis Take Off Polar Angle	0
SpcLbl	Species Label	Fe
TrnLbl	Transition Label	LMM
AbsLbl	Abssissa Label	kinetic energy
AbsStr	Abssissa Start	0
AbsEnd	Abssissa End	1200