Technical Report

The "Spectral Data Processor" for Windows 3.1, 95, 98, NT or OS/2 and The "SpecMaster Pro" Digital Database System of 35,000 XPS Spectra

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Abstract: The field of surface analysis by XPS is more than 30 years old. Until now, there have been only a few data tables of XPS binding energies that help users to analyze and identify the features and the peaks in high energy resolution XPS spectra of the main XPS signals. That limitation will start to disappear as databases of complete sets XPS spectra appear. In 1985, this author began to build a very unique "self-consistent" database of complete sets of "correlated" XPS spectra. The database contains sets of correlated spectra from many commonplace reference materials. To view or analyze the spectra in the database the user needs software that can be used to (a) view processed spectra that are stored in memory or (b) completely reprocess the spectra in the database. The "Spectral Data Processor" (XI-SDP) is a new Windows based software produced by XPS International, Inc., just for this purpose. This publication provides images of the software screens of the key features of the "XI-SDP" software and describes some features of the "XI SpecMaster Series of 35,000 Digital XPS Spectral Databases".

Introduction

The "SpecMaster Pro" Digital XPS Spectral Data-Base System includes advanced spectral data processing software, ASCII file format conversion, desk-top-publishing (DTP) capabilities, and most importantly a library of 35,000 digitized monochromatic XPS spectra.

This database is a unique "self-consistent" collection of spectra which were measured by a single scientist who collected all of the spectra over a 10 year time period by using two well-characterized SSI XPS systems equipped with Al K_α monochromatic X-ray sources.

The current collection of spectra is stored in 3,700 data-files which are organized as a modular system of 80 directories with names that are easily understood by analysts, engineers, scientists, and teachers. The entire collection is organized into two major libraries called the "Common Materials" and the "Practical Studies" Spectral Libraries, which are listed on the following two pages.

Each set of correlated spectra is designed to assist engineers, scientists, analysts, teachers, and theoreticians, who use XPS on an everyday basis under practical working conditions. These spectra are complete sets of correlated reference spectra that help XPS users to analyze industrial problems, gather reference data, perform basic research, test theories, and teach others.

The standard versions of the SpecMaster Series of spectral data-base systems are the *"SpecStarter", "SpecMaster Standard", and "SpecMaster Pro"* which can be customized to suit the needs of individual XPS users. (Ref 1)

The entire collection of spectra is designed to be a practical tool for everyday use and was obtained under practical working conditions. Although research grade spectra are not the main type of spectra in this system, there are, in fact, many thousands of research grade spectra in the database libraries. Research grade spectra are defined to be spectra obtained with high energy resolution, excellent charge control, and a high signal to noise ratio on a well calibrated system.

The "SpecMaster" digital XPS spectral database is a system that can be used in a practical manner on a daily basis by XPS users with many different needs and responsibilities.

The complete collection of spectra, which occupies about 200 MB of memory in binary form or about 400 MB in ASCII form, can be supplied on Laptop computer systems, on various types of magnetic, or optical recording media including for example: 2GB internal HDDs, 4 GB external SCSI HDDs, 100-1000 MB removable disks, 230-640 MB magneto-optical disks, and CD-ROMs.

For ease of use, the names of the directories and filenames are names that clearly identify the basic contents or the purpose of that directory or datafile. All of the names are very familiar to XPS users, analysts, engineers, scientists, and teachers.

SPECTRAL LIBRARY #1: "COMMON MATERIALS"

Directory Name	*Material Class*	*Number of Spectra*	*Number of Species*	*Number of Data-Files*
AC-AC	metal acetyl-acetonates (pressed pellets)	>150	19	>20
ACETATE	metal acetates (powders)	15	2	2
ALLOYS_1	metal alloys, steels {as rec'd & etched}	>500	44	>80
ALLOYS_2	metal alloys, steels - (part II)	>350	33	>60
ALUM-SIL	metal alumino-silicates (nat'l crystals)	>40	3	3
ANTISTAT	anti-static bag & coatings	40	6	6
BORIDE	metal borides (pressed pellets)	36	6	6
CALIBRAT	energy scale calibration spectra	>300	2	87
CARBIDE	metal carbides (pressed pellets)	40	3	5
CARBON	different forms of carbon	>120	13	>25
CARBONAT	metal carbonates (pressed pellets)	>150	15	>15
CATALYST	catalyst materials (new & used)	>170	15	28
CHALCOGN	chalcogenides (cleaved in air)	>80	9	12
CHROMATO	chromatographic materials (powders)	20	5	5
C_BLACK	carbon black materials (as rec'd)	30	9	9
C_FIBERS	carbon fibers (as rec'd)	13	5	5
DIAMOND	diamond related materials	50	10	12
ELEM_A-L	elements: Al-Lu	>450	48	>100
ELEM_M-Z	elements: Mg-Zr	>350	39	>50
FABRICS	fabric and cloth materials (as rec'd)	12	2	2
GLASS	glasses (cleaved in air)	>300	40	>50
GLOVE	contamination from gloves	>50	22	24
HALIDE	binary halides (crystals cleaved in air)	>100	10	>15
HYDROXID	binary hydroxides (pressed pellets)	60	8	9
MINERAL	natural minerals (crystals cleaved in air)	>400	36	45
MISC	miscellaneous materials	140	>25	>25
NITRIDE	metal nitrides (as rec'd & etched)	>100	6	>15
OXID_BIN	binary oxides (pressed pellets)	>900	80	>100
OXID_MIX	mixed oxides (cleaved or pressed)	120	>15	>15
OXID_NTV	native oxide films on elements (as rec'd)	200	41	41
OXID_REO	rare earth oxides (pressed pellets)	90	12	12
PAPR&INK	papers, fibers, and ink samples	>250	43	45
PHOSPHID	inorganic metal phosphides	>60	7	10
POLYMER1	organic polymers & polymer damage	>600	48	60
POLYMER2	polymers from NECSA\BIO group	100	30	100
PSG_SI	phosphorous silicate glass on silicon	58	9	9
REF_BE_1	reliable secondary reference energies	72	52	172
REF_BE_2	energy scale calibration for REF_BE_1	>300	2	80
RESIDUE	tap water residues	26	4	4
SEMICON1	semiconductor materials (cleaved/etched)	>650	>70	110
SEMICON2	semiconductor related materials	>450	48	70
SILICIDE	binary silicides (as rec'd & etched)	50	2	6
SULFIDE	binary sulfides (cleaved or pressed)	100	10	14
SUPERCON	superconductor materials (scraped)	80	5	15
SYSTMCHK	checks done on system behavior	250	3	96
TITANATE	metal titanates (cleaved in air)	31	3	4
TRANSMIS	spectrometer transmission studies	50	3	16
TUNGSTAT	metal tungstates (pressed or cleaved)	33	4	4
VB_ELEM	valence band data from elements	37	37	40
VB_OXIDE	valence band data from binary oxides	70	70	70
VB_SEMIC	valence band data from semiconductors	50	50	50
ZEOLITE	zeolites (as rec'd after treatments)	60	14	18

Numerical filenames, which add an unnecessary level of complication, were deliberately avoided.

To keep up with the ever growing needs of XPS and AES users, XPS International Inc. is working to update, expand, and improve the contents and features of the XI Library of XPS Spectra, and has developed a Windows based software called "Spectral Data Processor" (v2.0), which very easily converts and reads ASCII files from any of the major XPS systems. After importing ASCII data, the software can process the data and, very importantly, save all of the processed results to permanent memory.

Summaries of the Contents of the Two Major Spectral Libraries

The contents of the two major groups of spectra in the XI Library of XPS Spectra are divided into "Spectral Library #1: Common Materials" and " Spectral Library #2: Practical Studies". The "Common Materials" library is useful for analyzing and making assignments of commonplace materials. FWHM data are readily available from this library. The "Practical Studies" library has several functions. It is basically a tool for teaching others or yourself and is useful to study various real world techniques or avoid some real world problems.

Description of "Spectral Data Processor" Software

The "Spectral Data Processor" software (see Figure 1) is an advanced, Windows based, spectral data processing software that provides the processing features needed and wanted by XPS and AES analysts and scientists who work in many different fields.

The main features and capabilities of this software are presented here in a series of images (Figures 1-8). A detailed list of the features is beyond the limits of the current publication.

SPECTRAL LIBRARY #2: "PRACTICAL STUDIES"

Directory Name	*Practical Studies*	*Number of Spectra*	*Number of Species*	*Number of Data-Files*
ANGL-RES	angle resolved XPS	>200	10	50
CALIBRAT	energy scale calibration spectra	>300	2	87
CAPTUR_1	oxygen and carbon capture by metals	>2,800	42	44
CAPTUR_2	final condition from "captur_1"	23	17	17
CHRG_ALO	charge-up of aluminum oxide	>150	10	40
CHRG_C	charge-up of adventitious carbon	>200	15	>50
CHRG_GRZ	charge-compensation via grazing X-rays	120	5	30
CHRG_RES	charge-compensation research	>400	33	>120
DMG_ELEC	damage from flood gun electrons	>100	5	15
DMG_ION	damage from argon ion beam	90	12	25
DMG_XRAY	damage from monochromatic X-rays	>500	23	28
DPTH-PRO	depth profile examples	>8,000	43	>50
ELEMETCH	pure elements after long ion etch	>5,000	50	50
ETCHRATE	etch rate calibrations using SiO2	200	1	5
GAS-SNRS	carbon monoxide gas sensors	36	7	18
GLOVE	contamination from gloves	>50	22	24
GRAZINGX	enhanced count-rate from grazing X-rays	90	3	45
HD_LUBE1	line profiles of hard disk lubrication	70	14	50
HD_LUBE2	line profiles of hard disk lubrication	84	42	84
HEAT_EFF	effect of heat on materials	20	2	5
ION_IMPL	ion implanted materials (and profiles)	>600	12	30
LASERXPS	Laser-XPS research - part I	>650	44	318
MAG_MEM	magnetic materials	80	16	40
NTVOXFG1	effect of flood gun on native oxides	>300	24	>100
NTVOXFG2	effect of flood gun on native oxides	>250	21	>100
PELLET_R	research on making specimen pellets	40	7	12
SYSTMCHK	checks done on system behavior	250	3	96
TRANSMIS	spectrometer transmission studies	50	3	16
TRIBOLGY	tribology studies on bearings	50	6	15

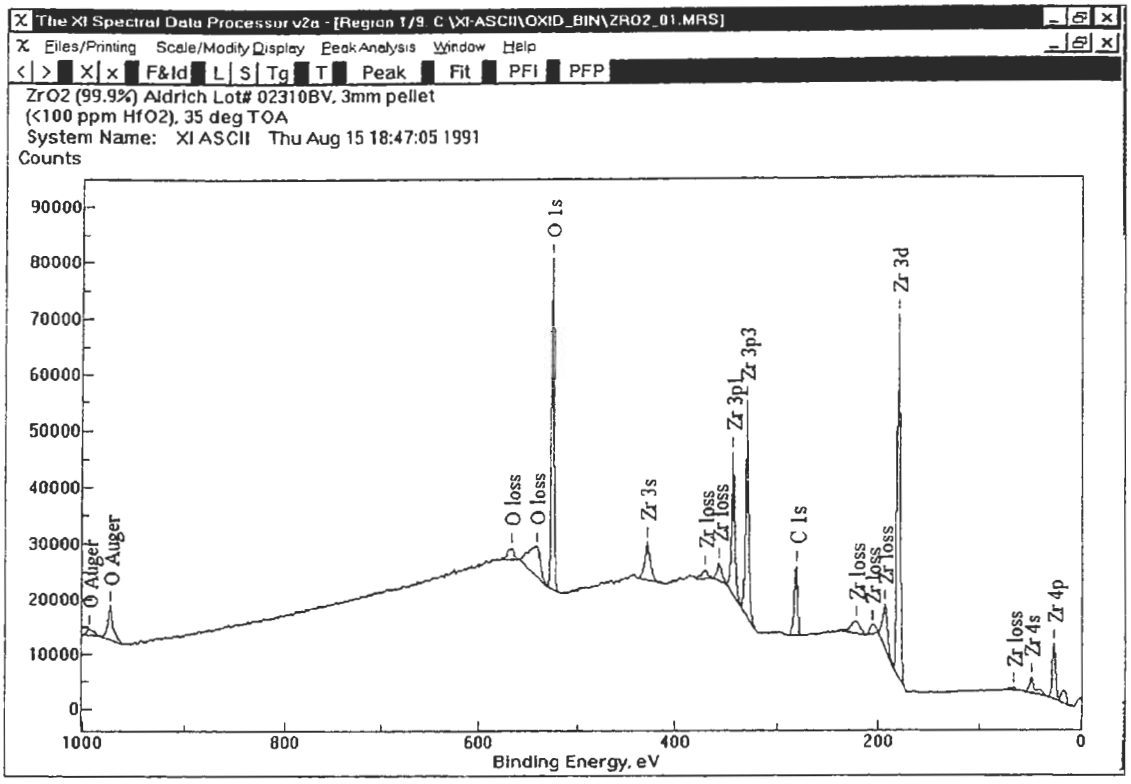

Figure 1. Main Menu of the XI SDP v2.0 software after identifying the peaks. In this figure you can see the peak areas that will be used to calculate atom percentages.

This software can import ASCII datafiles by simply dragging a single or multi-spectra ASCII datafile onto the open window of the XI-SDP software. After the spectra have been imported, the software is used to analyze and label the spectra. The software can save all peak-fits results, atom % results, and wide scan labels to permanent memory to be recalled at any time, which is just one of the advanced and user friendly features provided by this software.

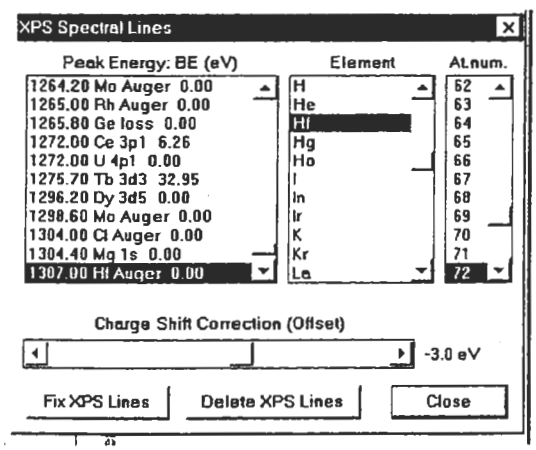

Figure 2. A Pop-Up menu that shows the "XPS Spectral Lines" routine that is used to identify the peaks that are present in wide scan and narrow scan spectra.

The pop-up window, called "XPS Spectral Lines" in Figure 2, has several ways of being used and is filled with 1,100 BEs derived from the pure element spectra in the XI Library of 35,000 XPS Spectra. This figure shows that the user is checking for the presence or absence of the element Hafnium (Hf).

The XPS Spectral Lines data table can also be used with the automated "Find & ID" routine which is a standard feature of the software.

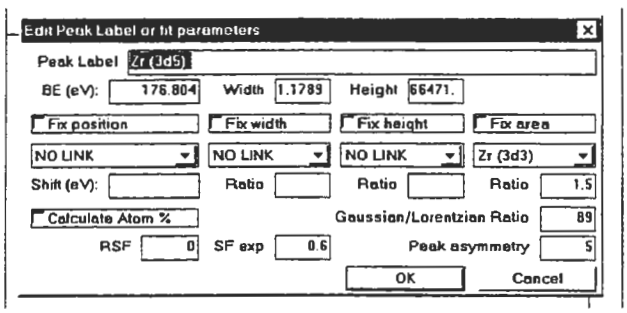

Figure 3. The pop-up menu shows the many controls that can be used to perform advanced peak-fitting.

In Figure 3, the reader can see the advanced peak-fitting capabilities provided by this sofware. The user can MODIFY, FIX (make constant) ,or make a RATIO of BEs, PEAK FWHMs, PEAK

HEIGHTS, and, most importantly, PEAK AREAS.

This figure shows that the user can assign a long name to any of the peaks. This is in addition to an "Annotation" function that allows the user to make annotations anywhere on the spectrum.

When a spectrum is printed, then the actual plot will contain the peak labels, the BEs, the FWHMs, the peak areas, the directory name, and the standard two lines of sample description.

In the "Edit Peak Label or Fit Parameters" pop-up menu shown in Figure 3 the user can modify any relative sensitivity factors (RSFs) by modifying the exponent factors of a simple polynomial algorithm that is designed to correct for transmission function effects or mean free path effects on the observed intensities of the XPS signals.

It is very easy to control the Gaussian / Lorentzian peakshape ratio and the degree of asymmetric tailing that is sometimes needed to properly analyze high energy resolution spectra.

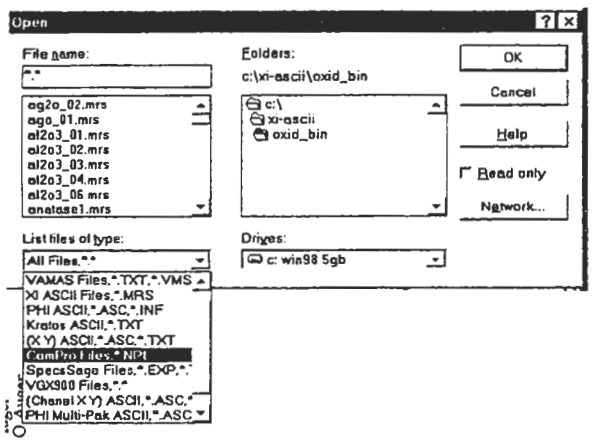

Figure 4. The "Open" file pop-up menu shows the many different ASCII file formats that are easily imported into the XI-Spectral Data Processor v2.0.

Figure 4 shows a partial list of the many different ASCII file formats that are currently supported. The SDP software also has the ability to import (X-Y) and (Channel X-Y) ASCII text files which is a very useful feature that allows users to import ASCII data from hand-made software, such as those made for operating analyzers that are connected to synchrotron systems or specialty XPS systems.

The ability to import the original VAMAS Standard Data Transfer Format is also provided. It can be used to import datafiles from that are produced by the ComPro software system.

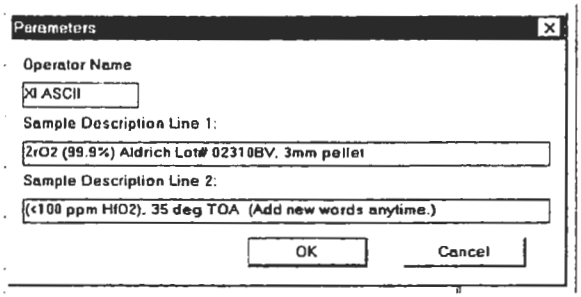

Figure 5. This figure shows a pop-up menu that allows the user to modify the two lines of "Sample Description" that are useful to record special details about the sample.

This menu shown in Figure 5 allows the user to add any important information or other details that were not added at the start of the analysis.

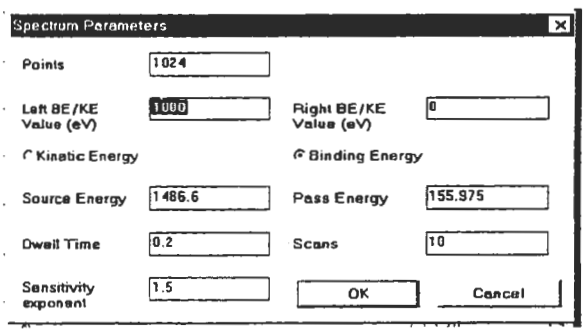

Figure 6. This figure shows the pop-up menu of the key "Spectrum Parameters" which can be modified at any time.

The ability to quickly review or modify the key spectrum parameters, shown in Figure 6, is very useful when comparing or analyzing data measured by using different XPS instruments.

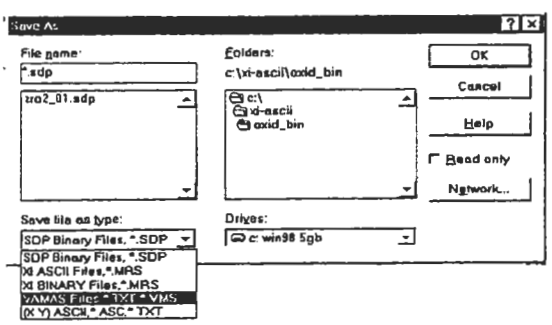

Figure 7. The SDP software can save any set of multiple spectra in several different file formats including the standard VAMAS DTF format and a simple "XY" format that can be read by many other data processing software.

When the user wants to save all the data processing results such as atom %, peak-fits, FWHM, and other very useful processing results to permanent memory, then the user must select the specially designed SDP Binary file that saves all of those important details to permanent memory. This is shown in Figure 7.

Figure 8 shows the ability to display several spectra at the same time by using "Tiling".

Some of the data processing features which are not shown in Figures 1-8 are:

(a) overlay of multiple spectra (4 different modes – normalized, proportional, offset)
(b) residual peak error in peak fit
(c) fitting Tougarrd baseline
(d) merge files or delete individual spectra
(e) print peak-fit details or atom % table
(f) multi-point smoothing or differentiation
(g) Un-Do last action
(h) adjust data by a fixed value (+ - / *)
(i) auto-scale of Y axis
(j) zoom with mouse or manual
(k) adjust page layout size
(l) control color and thickness of peak-fit lines

The SDP software will be further developed over the next few years so that it includes many more advanced data processing features and desk-top-publishing features which will be useful to XPS and AES users.

References

1. The SpecMaster series of databases are fully described in the XPSDATA.COM web site of XPS International.

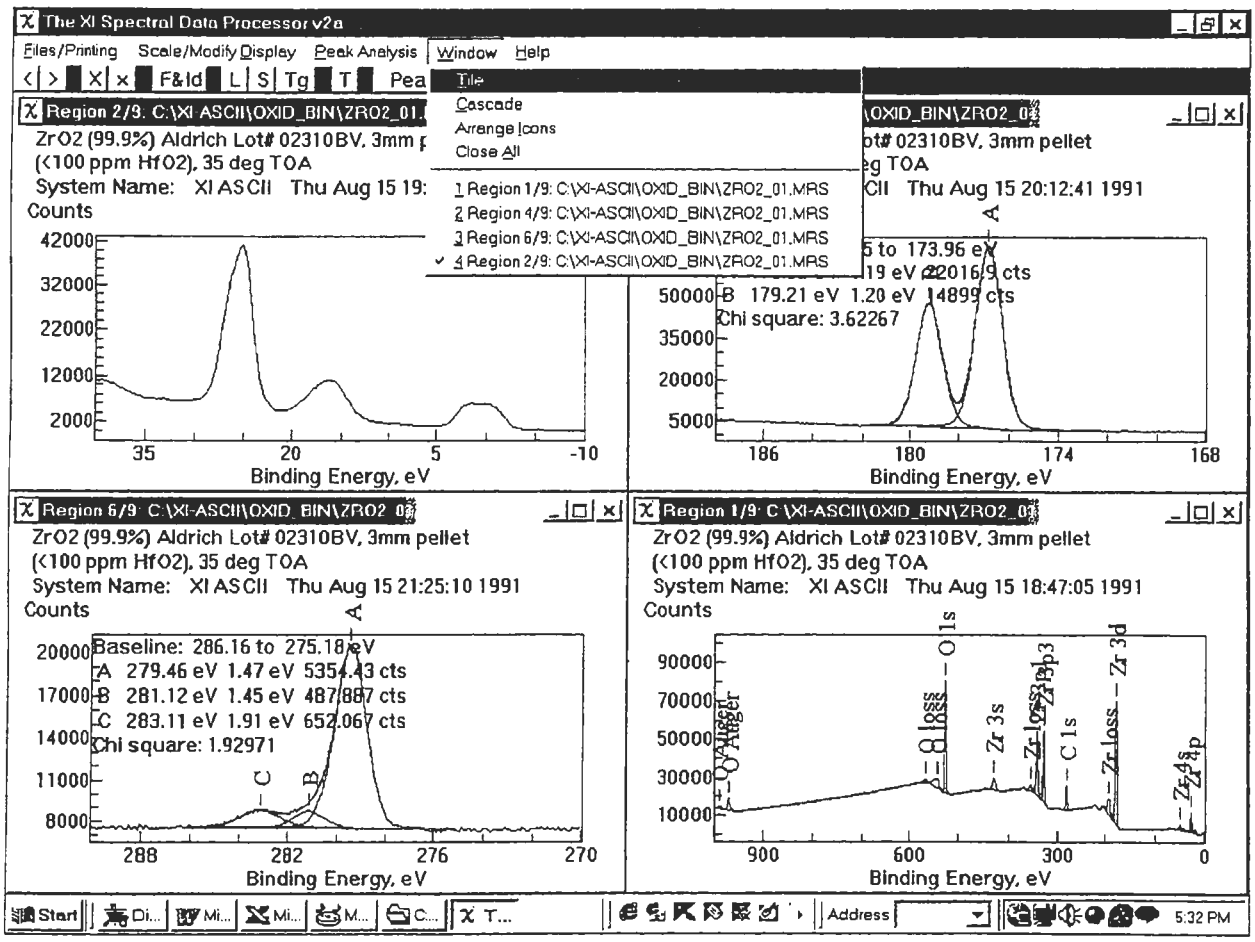

Figure 8. The ability to display multiple spectra on one page is called "Tiling". That feature is shown here in this figure because Tiling allows the user to compare a set of many different spectra from different data sets or the same data set or to make a useful 4 spectra plot for a report. This figure shows 4 spectra which were obtained from a sample of ZrO2.