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# XPS MultiQuant: a step towards expert systems

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**A thorough evaluation of photoelectron spectra is impossible without involvement of data systems. It is advantageous if the different programmes are easily able to communicate with each other. This connectivity may also serve as a base for future expert systems. The well-known VAMAS file format provides the first necessary step, converting the spectra into forms portable between various platforms.**

**In this paper, a new file format, the *XPS Reduced Data Exchange File*, is proposed, which defines an 'interface' between programs to transfer the derived XPS data.**

**XPS MultiQuant, which can be used routinely together with various spectrum processing packages to improve the flexibility and precision of quantitative calculations, is a typical target application requiring transfer of reduced experimental data (e.g., selected elements, line position, intensity data, etc.). The latest version of XPS MultiQuant already implements the *XPS Reduced Data Exchange Files* proposed here, to transfer necessary data between programs.** 

**KEYWORDS:** X-ray photoelectron spectroscopy; XPS; expert system; quantification; MultiQuant

## INTRODUCTION

X-ray photoelectron spectroscopy is one of the most powerful surface analytical techniques now available. As the fields of application of XPS are widening, more and more users with limited experience are being confronted with having to operate XPS systems. Thus, incorporation of 'expert' elements into the XPS data systems is inevitable in the future. Recently a workshop was devoted to the topic.[1] Although a 'complete' expert system is extremely complex, efforts have already been made to realize some elements of it.[2–5] The first step towards an expert system is to establish communication between the various existing XPS-related programs.

The typical data flow in an XPS system and outside is shown in Fig. 1. The data acquisition program controls the electronics of the instrument and collects data. The acquired data are usually stored in files with individual formats. Application of the programs supplied with the commercial instrument is usually inevitable because of the special requirements needed to control the spectrometers.

However, the programs for the spectral processing step can be selected, in general, without restrictions. Many of these programs can read numerous file formats but the well-known VAMAS file[6] provides a universal solution for transferring spectral data.

The data flow usually stops at this point, although transferring of the *reduced data* provided by the spectral processing components, including peak position, full width at half-maximum (FWHM), integral intensity, etc. seems to be a trivial task. Looking up line positions in a database,[7] calculating inelastic mean free path (IMFP) for the determined energies,[8] and performing special quantification[9,10] usually require manual transfer (i.e. reading and retyping) of data. Transferring large amounts of data this way is tedious and may be a potential source of errors.

In this paper, a new file format, the *XPS Reduced Data Exchange File*, is suggested, which defines an 'interface' between programs to transfer the derived XPS data.

## DISCUSSION

Although there are several advanced methods available for communication of programs running within one or different computers, a simple way, communication via unformatted character files with defined structure, was selected for the proposed task. It has several advantages: it can be applied within one computer or between two or more computers, and the latter can be done not only by networking but also by off-line media. In case of detection of computer read errors, the character file can be easily inspected by human reading.

### Data to transfer

The proposed file structure is focused on transferring data for quantification purposes but its application is not restricted to this field. Beside the trivial data, comprising of element symbols and electronic transition names, transferring of line energies, intensity values and other parameters is also advisable. These are the general parameters of the XPS measurements, like excitation energy, suggested cross-sections, sensitivity factors, etc. and data to identify measurements (data-set title and experiment labels).

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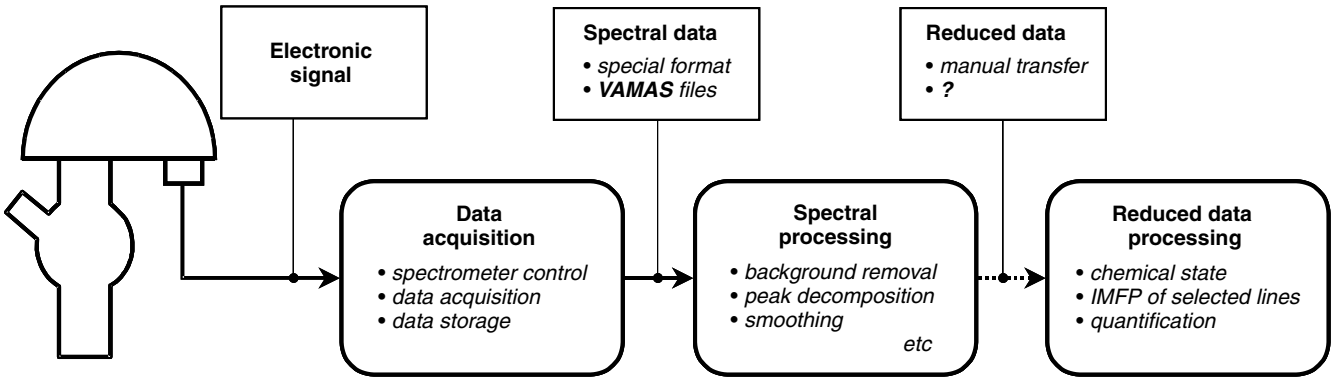


**Figure 1.** Data flow of an XPS data acquiring–processing system.

The data should be segmented into sections separating the general *Parameters, Elemental* and *Experimental* (*Intensity, Energy* and *FWHM*) data. This structure has several advantages: the file is compact because there are less redundancies, the compiled data is available in a 'matrix' form instead of a list, and, if the files are processed simply by a spreadsheet program, it is easier to select the required values for one element or one experiment.

## The proposed file format

The structure of the suggested file is shown in Fig. 2. The header line (XPSRDE) identifies the file type and its version. The presence of the version number enables further expansion of the exchange files with new features.

The *Title* keyword helps to identify the XPS quantification data set.

The *Parameter* section supplies various optional parameters of the XPS measurements. The keywords of this section give information on the applied excitation, cross-sections, IMFP, angular and contamination correction methods, analyser transmission and the selected experiment labels. The keywords can be present in any order within the section. This section and all of the parameters are optional. Instead of the missing parameters, default values should be provided by the target application. The number of selectable parameters is limited because the main purpose of this file type is to transfer large amounts of data between programs, although basic tasks, such as a simple quantification, can be invoked immediately. More sophisticated features (e.g. calculating IMFP by the TPP-2M or CS2 formulae or using complex quantification models) should be selected in the target applications; in this case interaction with the user is necessary.

```
XPSRDE  version
TITLE  title of data set

[PARAMETER]
[EXCITATION  mg|al|other energy]
[CROSS  none|scofield|evans|wagner|nefedov]
[IMFP  none|exp exponent|jablonski element|inorganic|polymer]
[ANGLE  none|reilman|ebel]
[TRANSMISSION  none|frr|fat|exp exponent|file filename]
[CONTAMINATION  none|evans|mohai]
[LABEL  {name|time|tilt|temperature}]
ELEMENT
{symbol line [state][b.e.][cross s.][asym.][at.w.][val.][ox.]}
INTENSITY
{{[label]} {intensity}}
[ENERGY
{{[label]} {energy}}]
[FWHM
{{[label]} {fwhm}}]
END
```

**Figure 2.** Structure of the XPS Reduced Data Exchange File using the Backuse-Naur Form (BNF) notation. Words appearing in **boldface** are keywords; in *italic* are parameters. Brackets enclose one or more optional items. A vertical bar separates alternatives. Items enclosed in braces can be repeated one or more times.

The *Element* section enumerates the elements and supplies basic quantification data for the XPS measurement given by the source application. In the element records the chemical symbol, name of the electron, energy level, chemical state, binding energy, cross-section, asymmetry parameter, atomic weight, valence and the number of oxygen atoms in an oxide are listed. Items of the element records are positional parameters, i.e. the separator of the omitted parameter must be present if there are any further parameters. All missing data will be replaced by the corresponding default value.

The *Intensity* section supplies the intensity data and the experiment labels of the XPS measurement. An experiment (also called *scan* or *level*) is a set of corresponding integrated photoelectron intensity data, e.g. intensities of the lines recorded after a step in an ion etch series. Items of the *Intensity* records are positional parameters, i.e. they should be treated as above.

The *Energy* section supplies the actual accurate line position data for each XPS experiment, which is suitable for chemical state determination. The energy values given in the *Element* section are *nominal* energy data only for transmission and IMFP approximation.

The FWHM section supplies the line width data for each XPS experiment. These values can be used to detect the presence of one or more chemical states, differential charging, etc.

Any of the *Intensity, Energy* or *FWHM* sections may be omitted from the *XPS Reduced Data Exchange File* but at least one of them must be present, depending on the purpose of the target application (e.g. a quantification application does not need FWHM data, a chemical state database does not need intensity values, etc.). The *experiment labels* are used either to identify experiments or to supply additional




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information, e.g. the ion etch time or tilt angle, etc. The content of labels in the *Experiment* sections must be the same because the target application may process only one of them.

The *End* keyword terminates the file.

## Source and target applications

Source applications providing the *XPS Reduced Data Exchange Files* would include the XPS spectral processing software packages. Authors are encouraged to use this output format to improve connectivity of their programs. A detailed manual can be downloaded from the Internet.[11] A special test Reader program is also available to rigorously check the syntax of the exchange files and analyse possible errors (Fig. 3). There is already a promise that this file format will be included in the future version of some XPS software.[12,13]

Target applications may include all post-processing programs, like quantification, chemical state databases, spreadsheet and charting programs. The target applications of the *XPS Reduced Data Exchange Files* (including XPS MultiQuant) should be designed to read files prepared on various computer systems, if possible without any previous conversion.

- *Character encoding*: The XPS Reduced Data Exchange Files are usually simple ASCII files, but files with Unicode Little Endian, Unicode Big Endian and UTF-8 encoding can be also read.
- *Line terminators*: Line terminator characters can be LF (linefeed), CR (carriage return) and CRLF characters; thus files written under DOS, Windows, Unix, Linux and Macintosh operating systems can be read.
- *Decimal separators*: The decimal separator character can be either a dot or a comma, regardless of the current locale settings. However, use of digit grouping symbols should be avoided.
- *Item separators*: The item separator character can be TAB (tabulator) or semicolon.
- *Keywords and parameters*: All keywords and parameters are case insensitive. Usually the first four characters are significant, except the header, and when the keyword is less than four characters.

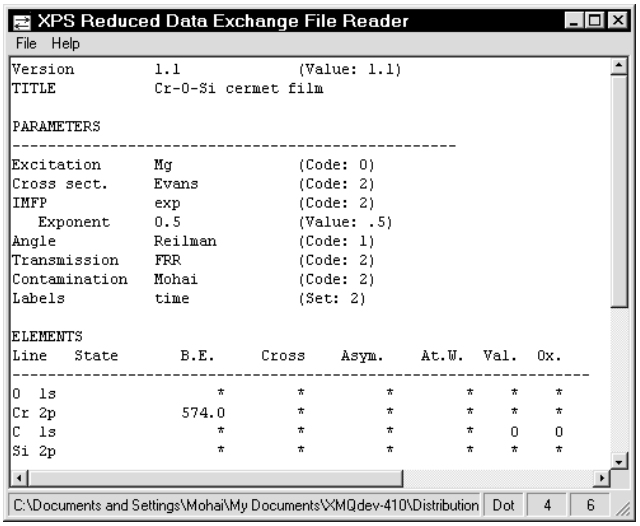


**Figure 3.** The test Reader program analyses the syntax of the XPS Reduced Data Exchange Files.

## Putting into practice: XPS MultiQuant

XPS MultiQuant is a stand-alone quantification program which can be used routinely together with spectrum processing packages to improve the flexibility and precision of quantitative calculations. It can also be applied for sophisticated calculation of layered samples (including its unique curved surface models[14]). The program uses the 'classic' approach of quantification, requiring the integrated intensities of the XPS lines. All usual correction methods and factors can be applied and controlled independently. The basic data for calculations are integrated into the library of the program. The results can be presented in various forms.

Interpreting of *XPS Reduced Data Exchange Files* has already been fully implemented in XPS MultiQuant. Files can be opened like standard data files or the source application can run XPS MultiQuant directly and pass the filename as a parameter. Transferring of data can be routinely applied for simple quantification, ion etch depth profiles, etc. and it gives immediate results. The advanced features of XPS MultiQuant (layer thickness calculation on flat or curved surfaces, sophisticated IMFP calculations) cannot be addressed directly by the *XPS Reduced Data Exchange Files* because these features require deeper interaction of the user anyway.

# CONCLUSIONS

- The described *XPS Reduced Data Exchange File* provides a simple way to communicate between spectral processing and post-processing programs.
- Data can be exchanged between systems running on different platforms without further conversion.
- The format is flexible and can be expanded later as required.
- Latest version of XPS MultiQuant is ready to read *XPS Reduced Data Exchange Files*.

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