User's Guide

# QUASES-Tougaard

## Quantitative Analysis of Surfaces by Electron Spectroscopy

Version 5.1

Software for Quantitative XPS/AES
of Surface Nano-Structures by
Analysis of the Peak Shape and Background

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# Contents

# Introduction.

A new method for non-destructive analysis of the 3 dimensional nano-structure of surfaces by XPS and AES was developed during the past years [1-8]. The analysis relies on algorithms that take into account the peak intensity, the peak shape and the background of measured energy spectra. In several recent experimental studies, the method has been demonstrated to give a much more complete and reliable picture of the quantitative composition of the surface region of the solid in comparison to traditional analysis, which relies exclusively on the peak intensity.

Several research- and surface analysis groups have expressed interest in a user friendly software package that could make these new ideas easily available.

To meet this demand, it was therefore decided to develop and market a software package.

QUASES™ (Quantitative Analysis of Surfaces by Electron Spectroscopy) is the result of this effort.

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The scientific basis for the software was published in these papers:

1) S. Tougaard, Surface and Interface Analysis, 11, 453 (1988)
2) S. Tougaard, Surf. Sci. 216, 343 (1989)
3) S. Tougaard and H. S. Hansen, Surface and Interface Analysis 14, 730 (1989)
4) S. Tougaard, J. Electron Spectr. 52, 243 (1990)
5) S. Tougaard, J. Vacuum Science and Technology A14, 1415 (1996).
6) S. Tougaard, Surface and Interface Analysis 26, 249 (1998).

# *Chapter 1*

## 1. Concept of the QUASES™ analysis procedures

This chapter describes the principle of analysis used in QUASES-Analyze and QUASES-Generate.
If you are already familiar with the ideas behind QUASES you can skip this chapter and continue in Chapter 2.

### 1.1 Introduction.

Quantitative surface chemical composition analysis by X-ray photoelectron or Auger electron spectroscopy (XPS or AES) relies on several factors [1-3] like for example knowledge of photoionization cross sections, inelastic electron mean free paths, and the influence of elastic electron scattering. The most serious problem in quantitative XPS, that gives the largest contribution to errors of analysis, is however assumptions made on the in-depth distribution of atoms. This is so because the measured peak intensity may well vary by orders of magnitude depending on the in-depth profile. As a result, a meaningful interpretation of measured XPS-peak intensities can not be made unless the in-depth distribution of atoms is known. Such information is however usually not at hand in practice, because it is the purpose of the analysis to find the quantitative composition of the surface region of the solid, and if this information were available there would be no point in doing the analysis. To be able to extract quantitative information from a measured peak intensity, it is necessary to make an assumption, and for convenience it is usually assumed that the surface region is homogeneous up to a depth of a few nano-meters. This assumption does however make quantification of surface chemical compositions by XPS and AES extremely unreliable as shown below.

In view of the high and rapidly growing technological importance of reliable information on the in-depth composition of the surface region of solids on the nano-meter scale, much effort has in recent years been devoted to the development of new more accurate methods. With this goal in mind, Tougaard et al [3-8] has made systematic studies of electron transport phenomena and on this basis developed a practical technique for determination of the chemical composition of solid surfaces with nano-meter depth resolution. It relies on the phenomenon that the energy loss structure that accompanies an XPS or AES peak carries information on the depth of origin of the detected electrons. The method is non-destructive and therefore allows also studying the change in surface morphology during exposure to various treatments as, e.g., gradual annealing or chemical reaction with an ambient gas. The technique has been applied to study thin film growth mechanisms and inter-diffusion depth profiles of many systems including also several tests on the validity of the method (see ref.[8] and references in ref.[8]).

The QUASES™ software package provides a practical tool that makes application of these results possible for routine analysis work.

## 1.2 Quantification with Peak Intensities. Errors and Uncertainties.

For a meaningful quantification of measured peak intensities, assumptions on the in-depth distribution of atoms must be made. Usually, the sample composition is taken to be homogeneous up to a depth of a few nano meters [1]. This assumption may result in enormous errors in quantification [6-8]. Thus, solids subject to surface analysis are hardly ever homogeneous up to a depth of several nano-meters. It is precisely because samples are *inhomogeneous* on the nano-meter depth scale that analysis is done with XPS or AES rather than with other well-established methods for chemical analysis that are less surface sensitive

The reason for the dramatic change in peak shape with the surface morphology is that as the electrons move on their way out of the solid, they lose energy. The longer pathlength they travel, the larger is the fraction of the electrons that have lost energy. This is illustrated in fig.1.1 where the energy spectrum is shown before and after the electrons have passed a thin solid with different thickness. For electrons that pass only a short distance in the solid, the chances that an electron will lose energy is small and the change in energy distribution is small. For electrons that pass a larger distance, a larger fraction will have lost energy and the intensity at the peak energy is diminished. These electrons are found at lower energies in the spectrum and the distortion of the energy spectrum is substantial.

The formula mostly applied for quantitative analysis by XPS and AES relies on the assumption that the average concentration in the outermost surface region of the solid is directly proportional to the measured peak intensity. To illustrate the fundamental problem with this procedure we will consider an example of model spectra calculated for different depth distributions of copper in a gold matrix. Thus, fig.1.2 shows spectra of the Cu2p peak corresponding to four different surface morphologies. The XPS-peak intensity from all four solids is exactly identical although the surface morphologies are widely different. Quantification based only on the Cu2p peak intensity cannot discriminate between these four structures. Analysis of these spectra under the assumption that the surface concentration is proportional to the peak intensity, would then result in a quantification where the concentration at the surface could be anywhere from 0 % (as in (d)) to 100 % (as in (a)). The total amount of copper material within the surface region could be anywhere from the equivalent of 1.1 Å (as in (a)) or 10 Å as in (c)) or even higher (as in (d)). Quantification based on peak intensities alone is thus subject to extremely large uncertainties and it is hard to keep the imagination of XPS and AES as quantitative techniques.

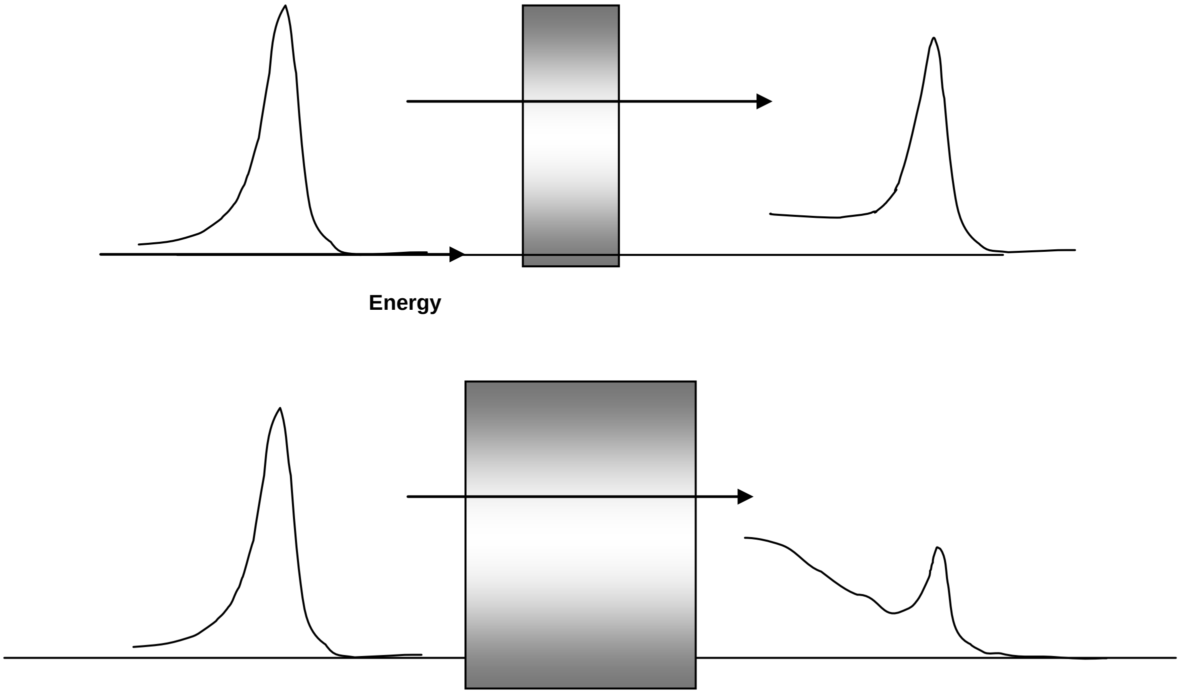
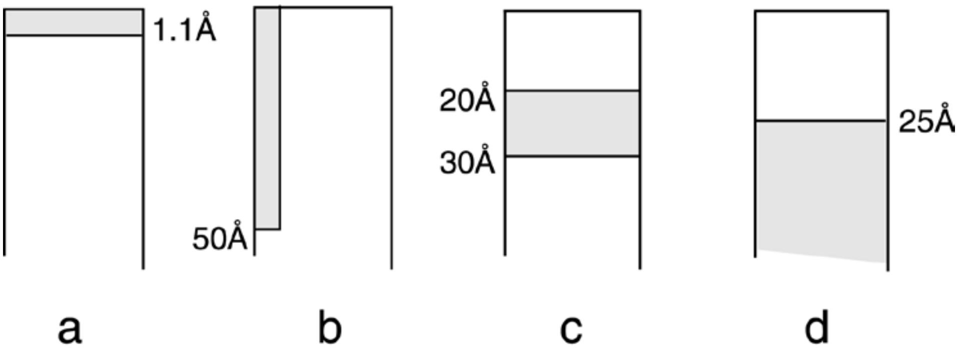


**Figure 1.1**



These surface morphologies all give the same XPS-peak intensity

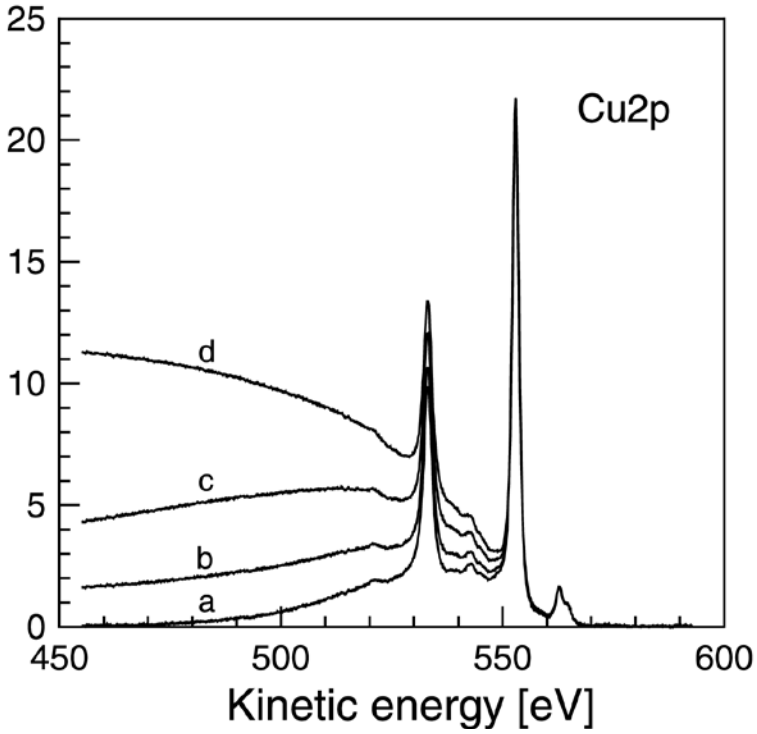


**Figure 1.2**

On closer inspection of the spectra in fig.1.2, it is clear that the peak shape in a wider energy range below the peak does depend critically on the in-depth distribution of the element. It is thus easy experimentally to distinguish between the peak shape of the four spectra in a say ~ 100 eV energy region. Much more accurate quantification can therefore be accomplished if the dependence of peak shape on surface morphology is taken into account in the analysis. It is a quantitative description of these effects that is the basic principle of surface nano-structure quantification in QUASES™.

In fig.1.2 (a), the electrons have traveled only a short distance before they escape through the surface, and consequently, very few have lost energy and the intensity on the low energy side of the peak is small. In Fig1.2 (c), all electrons have traveled ~20-30 Å within the solid before they reach the surface, and a larger fraction have lost energy and end up at lower energies in the spectrum. In fig.1.2 (d), there are additional electrons coming from larger depths, and these electrons will have lost further energy. This is why the intensity ~ 50 – 100 eV below the peak is considerably larger in (d) compared to (c).

## 1.3 Quantification with QUASES™.

This section briefly summarizes the principles used in QUASES™ to describe the variations in energy distribution of emitted electrons caused by electron transport.

The flux density of photoelectrons excited from a single atom at energy $E_0$ into the solid angle $\Omega$ is denoted $F(E_0,\Omega)$ and the concentration of atoms at depth x is f(x).
Then the measured spectrum of emitted electrons is

$$J(E,\Omega)=\int dE_0\, F(E_0,\Omega)\int f(x)G(E_0, x/\cos\theta;E)\, dx \qquad (1.1)$$

where θ is the emission angle with respect to the surface normal. The function G, is the energy distribution of an electron as a function of path length x/cosθ traveled in the solid.

The total energy loss of an electron moving in a solid is determined by the inelastic scattering cross section and the path length traveled. Multiple scattering events are important because in typical cases, the energy spectrum includes electrons that have traveled a distance of several inelastic mean free paths.

We denote by K(E,T) the differential inelastic electron scattering cross section, i.e. K(E,T)dRdT is the probability that an electron of energy E will lose energy in the interval T, T+dT after having traveled a path length dR in the solid. For energy spectra where the total energy loss is small compared with the primary electron energy, K(E,T) ≅ K(T) independent of E. Then the effect of multiple scattering has a rigorous solution, and the spectrum of emitted electrons is

$$J(E,\Omega) = \int dE_0\ F(E_0,\Omega) \int ds\ \ e^{-i\,2\pi s\,(E-E_0)} \int dx\, f(x)\, e^{-x\,\Sigma(s)\,/\cos\theta} \qquad (1.2)$$

with

$$\Sigma(s) = \frac{1}{\lambda_i} - \int_0^\infty K(T)\, e^{-isT}\, dT \qquad (1.3)$$

where λ is the inelastic electron mean free path.

## Quantification by Background Removal.

Formulae to determine the atomic excitation function F(E, Ω) from a measured spectrum were developed for different types of in-depth profiles. It was shown that the integral equation (eq.(1.2)) may be solved rigorously for the primary excitation spectrum F(E, Ω)

$$F(E,\Omega) = \frac{1}{P_1}\left[ J(E,\Omega) - \int dE' J(E,\Omega) \int ds \exp\left[i 2\pi s(E' - E)\right](1 - \frac{P_1}{P(s)}) \right] \qquad (1.4)$$

where

$$P(s) = \int dx\, f(x) \exp\left(-\frac{x}{\cos\theta}\Sigma(s)\right) \qquad (1.5)$$

and

$$P_1 = \int dx\, f(x) \exp\left(-\frac{x}{\lambda_i \cos\theta}\right) \qquad (1.6)$$

Eq.(1.4) may be used to determine either F(E, Ω) if *f*(*x*) is known (e.g., for a one elemental sample) or it may be used to determine *f*(*x*) if F(E, Ω) is known. The exact peak shape in the energy region close to the peak energy up to ~ 10-20 eV below the peak energy is not known since it is largely determined by the chemical bond, lifetime broadening, and intrinsic excitations in the photoemission process which all may depend on the local chemical environment. However, the spectrum F(E, Ω) after background correction must be of zero intensity in an energy region beyond ~ 30eV below the primary peak energy and the spectral intensity must stay at zero intensity for all energies below the peak energy until the energy of another peak in the energy spectrum is reached. This puts a strong constraint on the function F(E,Ω) and this is applied as a criterion to determine *f*(*x*) in the sense that *f*(*x*) is varied until the constraint is fulfilled.

As another criterion one can use knowledge about F(E,Ω) determined from the analysis of spectra from samples with a well characterized in-depth concentration profile as, e.g., a single element solid. One should be aware of the possible peak shape changes caused by the difference in chemical environment of the atoms in the reference and the sample being investigated. To the extent that these differences can be neglected, the spectrum may be applied as a reference and *f*(*x*) is varied until analysis yields a spectrum with the same absolute intensity and peak shape as the reference spectrum. If the peak shape analysis includes peaks from all the elements in a sample then the constraint that the sum of the concentration of the individual elements at any depth must add up to 100% may also be applied.

## 1.4 Inelastic electron scattering cross sections

The cross section K(T) can be described with sufficient accuracy by Universal formulas valid for different classes of materials.

Depending on the class of materials, a function with either two, or three parameters is needed to describe the cross sections of that class [9].

For most metals, their oxides and alloys, the *Universal cross section* [9]

$$\lambda_i(E)K(E,T) \ = \ \frac{B\,T}{\left(C \ + \ T^2\right)^2} \tag{1.7}$$

with C= 1643 $\mathrm{eV}^2$ and B $\cong$ 3000 $\mathrm{eV}^2$ applies with sufficient accuracy.

For solids with a narrow plasmon structure, the cross-sections can not be well described by a function with two-parameters. For these however it was shown [9] that the main characteristics of the cross section can be described by the *Three-parameter Universal cross section*

$$\lambda(E)K(E,T) = \frac{BT}{\left(C - T^2\right)^2 + DT^2} \tag{1.8}$$

where the three parameters B, C, and D have been determined for each class of materials (e.g. polymers, semiconductors, free-electron-like solids [9]).

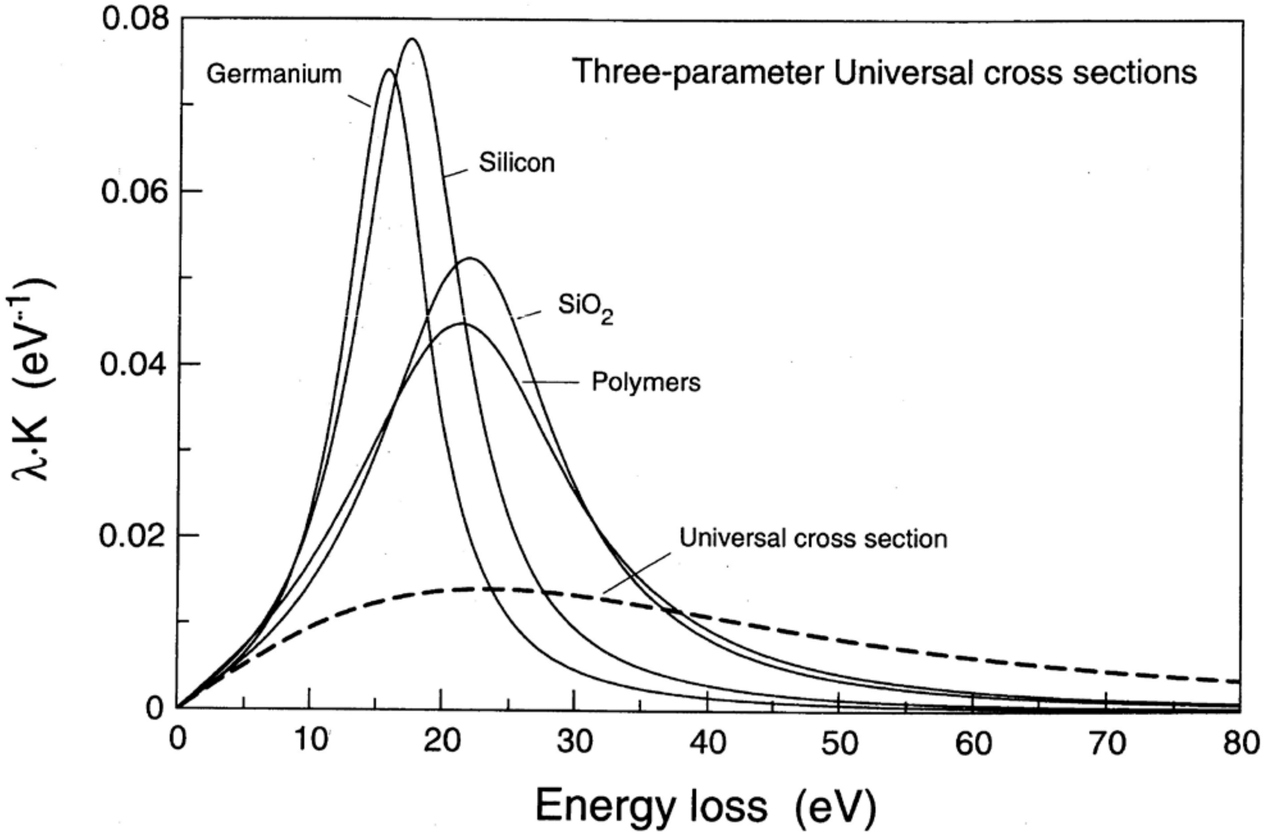

Three-parameter Universal cross sections
Germanium
Silicon
$SiO_2$
Polymers
Universal cross section
λ·K (eV⁻¹)
0.08
0.06
0.04
0.02
0
0
10
20
30
40
50
60
70
80
Energy loss (eV)

**Figure 1.3**

Fig 1.3 shows cross sections for various types of solids. The parameter values are given in table1. These cross sections are all included in the QUASES™ software.

**TABLE 1.** Parameters for the Universal cross sections in eqs.(1.7) and (1.8). $B^N$ is the value of B for which the cross section is normalized. Some of the cross sections are plotted in Fig. 1.2 and 1.3

**UNIVERSAL CROSS SECTION (EQ.(5))**

| Class of materials | B [$eV^2$] | $B^N$ [$eV^2$] | C [$eV^2$] |
|---|---|---|---|
| Metals and their oxides | 2866 | 3286 | 1643 |

**THREE PARAMETER- UNIVERSAL CROSS SECTION (EQ.(6))**

| Class of materials | B [$eV^2$] | $B^N$ [$eV^2$] | C [$eV^2$] | D [$eV^2$] |
|---|---|---|---|---|
| Polymers | 434 | 396 | 551 | 436 |
| Silicon-dioxide | 325 | 299 | 542 | 275 |
| Silicon | 132 | 131 | 325 | 96 |
| Germanium | 73 | 93 | 260 | 62 |
| Aluminum | 16.5 | 21.4 | 230 | 4.5 |

## References

1 M. P. Seah, in Practical Surface Analysis Vol. 1 Chapt. 5, (Eds., D. Briggs and M. P. Seah, Wiley, New York, 1990)

2 M. P. Seah, Surf. Interface Anal. 2,222 (1980) ,

3. S. Tougaard, Surface and Interface Analysis 11, 453 (1988).

4. S. Tougaard and H.S. Hansen, Surface Interface Analysis 14, 730 (1989).

5. S. Tougaard, J. Electron Spectroscopy 52, 243 (1990).

6 S. Tougaard, J. Vacuum Science and Technology A8, 2197 (1990).

7 S. Tougaard, J. Vacuum Science and Technology A14, 1415 (1996).

8 S. Tougaard, Surface and Interface Analysis 26, 249 (1998).

9 S. Tougaard, Surface and Interface Analysis 25, 137 (1997).

# *Chapter 2*

# Installing and Running QUASES

## System Requirements

- A PC with 80486 or higher processor (Pentium 133MHz or higher is recommended), running Microsoft Win 95 or Win 98 or Win NT.
- A CD-ROM disk drive for installing QUASES.
- A harddisk with 15 MB free disk space.
- VGA graphics 600x800 (1024x768 is recommended).
- A mouse

## 2.1 Installing QUASES-Analyze and QUASES-Generate

The QUASES™ software package consists of the two programs QUASES-Analyze and QUASES-Generate.
In QUASES-Analyze, the spectra are analyzed by removing the background of inelastic scattered electrons from the spectrum.
In QUASES-Generate, the spectra are analyzed by calculating the background of inelastic scattered electrons and comparing such model spectra to a measured spectrum.

### To install QUASES- Analyze:

1. Insert the compact disc in the CD-ROM drive.
2. Open the directory **Install Analyze**.
3. Click **Setup**.
   This starts installation of **QUASES-Analyze**. Follow the instructions on the screen.

### To install QUASES- Generate:

1 Insert the compact disc in the CD-ROM drive.
2 Open the directory **Install Generate**.
3 Click **Setup**.
    This starts installation of **QUASES-Generate**. Follow the instructions on the screen.

**Note**: The program assumes that the American standard for numbers is used and will not run properly if setting is different. To change settings, select *Start* on the Windows menu bar and then select *Settings, Control Panel, Regional Settings, English(United States)* or change the number settings for your current Regional settings to the American standard.

The directory PROGFILE contains setup files for the different classes of in-depth concentration profiles treated by the program. These files are automatically updated to contain the parameters for the last selected setup for each of the profiles. *Note: The user should not make any changes in the files in directory PROGFILE, since these are read by the programs and improper data may cause the programs not to run.* Reinstall the program if these files are accidentally changed.

## 2.2 Starting and using QUASES.

You can start QUASES-Analyze or QUASES-Generate by using the Start button on the task bar in Windows 95.

## Quantitative XPS by Peak Shape Analysis.

As was discussed in Chapter 1, there are two different approaches to the application of QUASES:

**In QUASES-Analyze**, the inelastic background is removed from the measured spectrum by formulae that depend on the in-depth concentration profile $f(x)$.

**In QUASES-Generate** the peak shape of the spectrum of emitted electrons is calculated by formulae that depend on the in-depth concentration profile $f(x)$. These model spectra are compared to the measured spectrum.

These procedures are briefly described below in Secs. 2.2.1 and 2.2.2.

### 2.2.1 QUASES-Generate. Quantification by Peak Shape Calculation.

In this approach, the spectrum $J(E,\Omega)$ is calculated by eq.(1.2) or by equivalent formulae that start with the spectrum from a pure elemental solid. The in-depth concentration profile $f(x)$ is then varied until a good agreement with the measured spectrum is obtained. In this way, the detailed in-depth concentration profile $f(x)$ is determined.

### 2.2.2 QUASES-Analyze. Quantification by Background Removal.

In this approach, the primary atomic spectrum $F(E,\Omega)$ is calculated by eq.(1.4) from the measured spectrum $J(E,\Omega)$. The in-depth concentration profile $f(x)$ is varied until the background has been removed in a large energy region below the peak energy. A reference atomic spectrum may also be applied, in which case the in-depth concentration profile is changed until a good match to both shape and intensity of the reference is obtained.

# *Chapter 3*

# Preparing spectra for QUASES analysis.

## Correct

**Note:** The programs assume that the American standard for numbers is used (where the decimal place is marked by a ".") and will not run properly if setting is different. To change settings, select Start on the Windows menu bar and then select Settings, Control Panel, Regional Settings, English (United States) . Alternatively, you may change the number settings for your current Regional settings to the American standard.

**This program is available in both QUASES-Analyze and QUASES-Generate.**

The purpose of the program **Correct** is to isolate the individual peaks of the spectrum before further analysis with QUASES-Analyze or QUASES-Generate. It corrects the measured spectrum for the following two effects:

- Energy dependence of the electron spectrometer transmission.
- The continuous background signal from peaks at higher energies.

Click **Correct** (see Fig.3.1) and get Fig3.2. In the filelist, click the name of the file with the spectrum you want to correct ( AG_AL). This causes the spectrum to be plotted (see fig. 3.2).

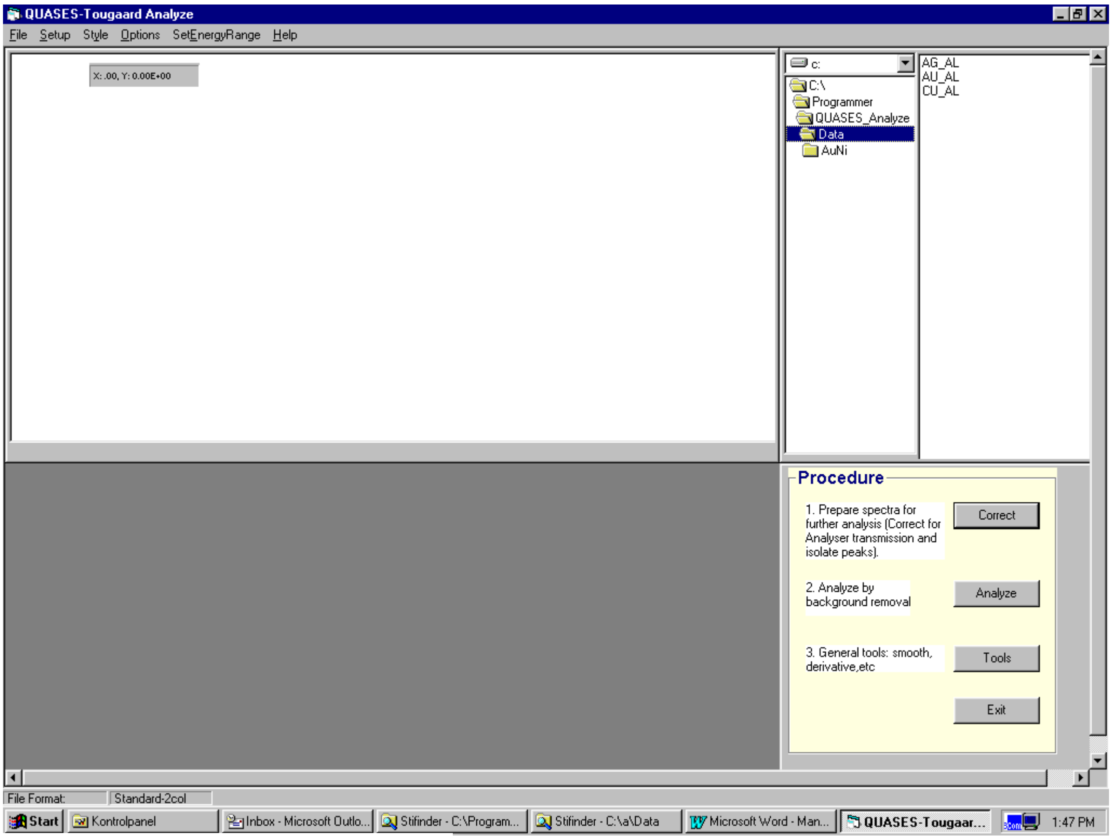
### Correct for electron spectrometer transmission

Now click the **TransmCorrect** button and get Fig.3.3. There are two options for correcting the spectrum for the energy dependence of the analyzer transmission.

**Function**

Select this option if the transmission function can be approximated by a power law (see fig.3.4). Click the textbox and type the value of m for the spectrometer. The subsequent QUASES analysis is not very sensitive to the chosen value and m=0.7 is a typical value valid with sufficient accuracy for most hemispherical analyzers when operated in the constant pass energy mode in the energy range of most XPS peaks. This value is recommended if no knowledge is available for the actual spectrometer transmission function. Click OK and get Fig.3.5.

The plotted spectrum has been corrected for the energy dependent transmission function.



**Procedure**

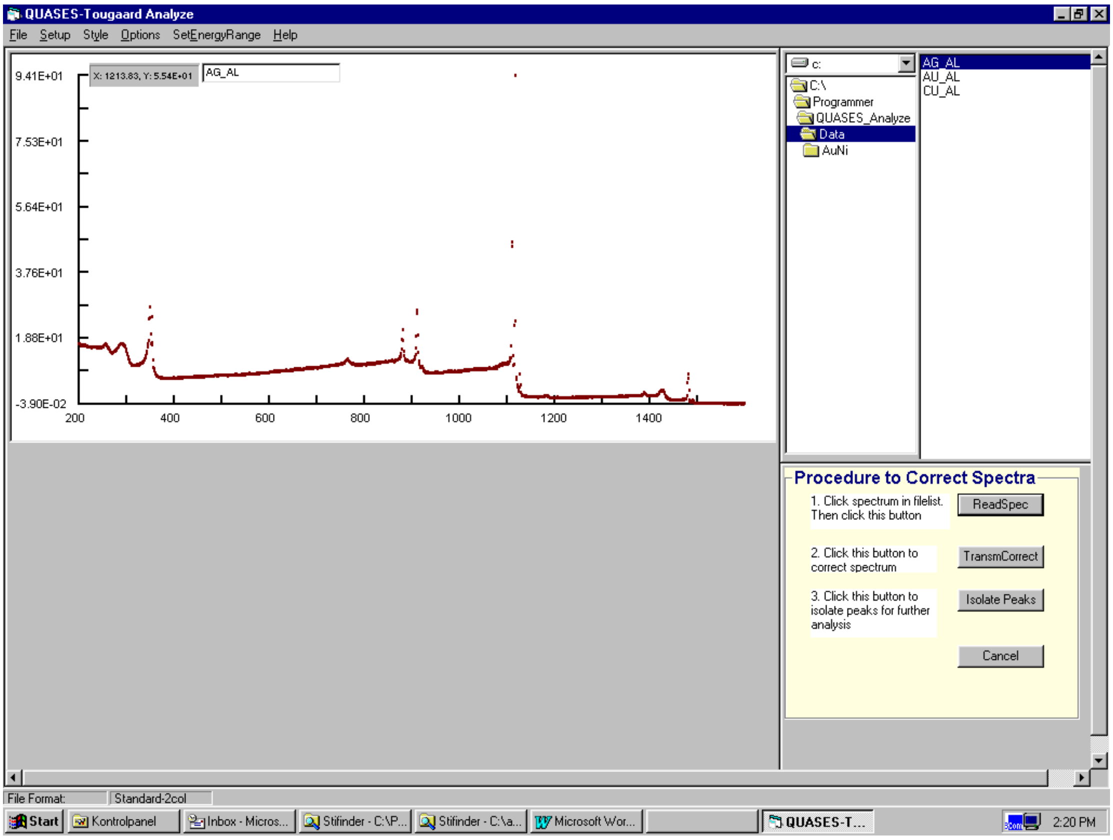
1. Prepare spectra for further analysis (Correct for Analyser transmission and isolate peaks).

2. Analyze by background removal

3. General tools: smooth, derivative,etc

File Format: Standard-2col

**Figure 3.1**



**Procedure to Correct Spectra**

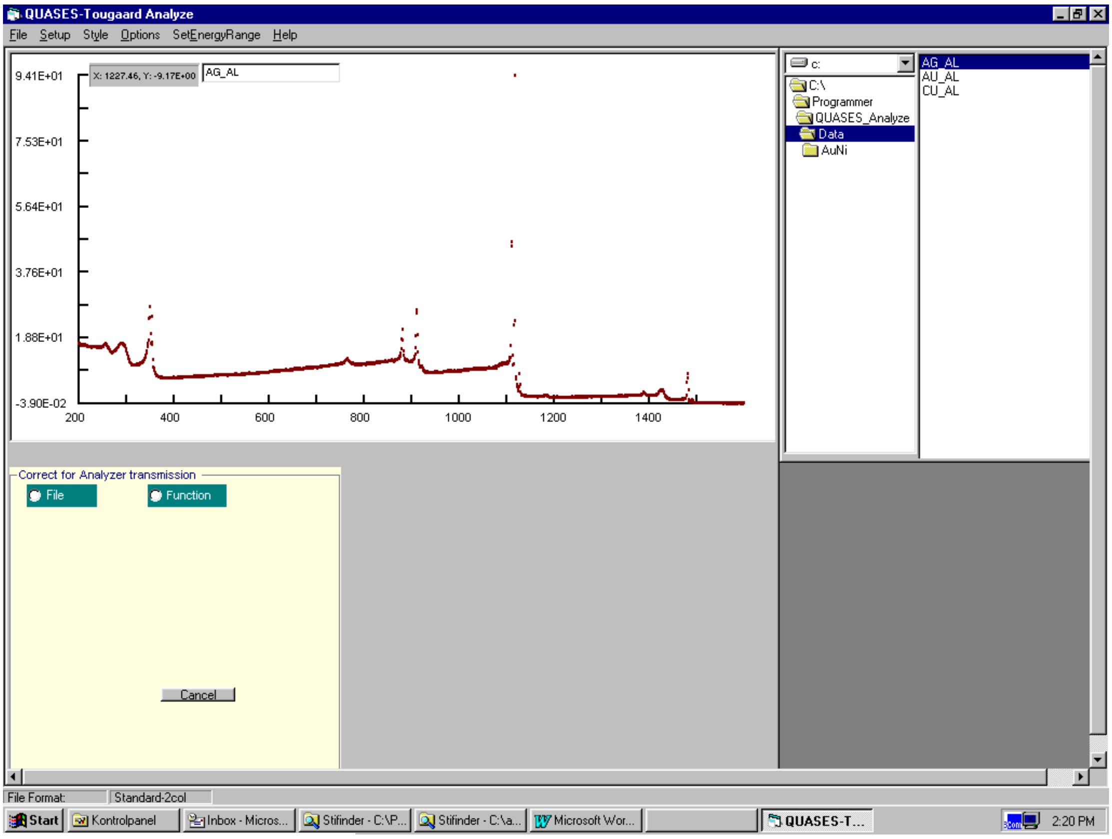
1. Click spectrum in filelist. Then click this button

2. Click this button to correct spectrum

3. Click this button to isolate peaks for further analysis

File Format: Standard-2col

**Figure 3.2**

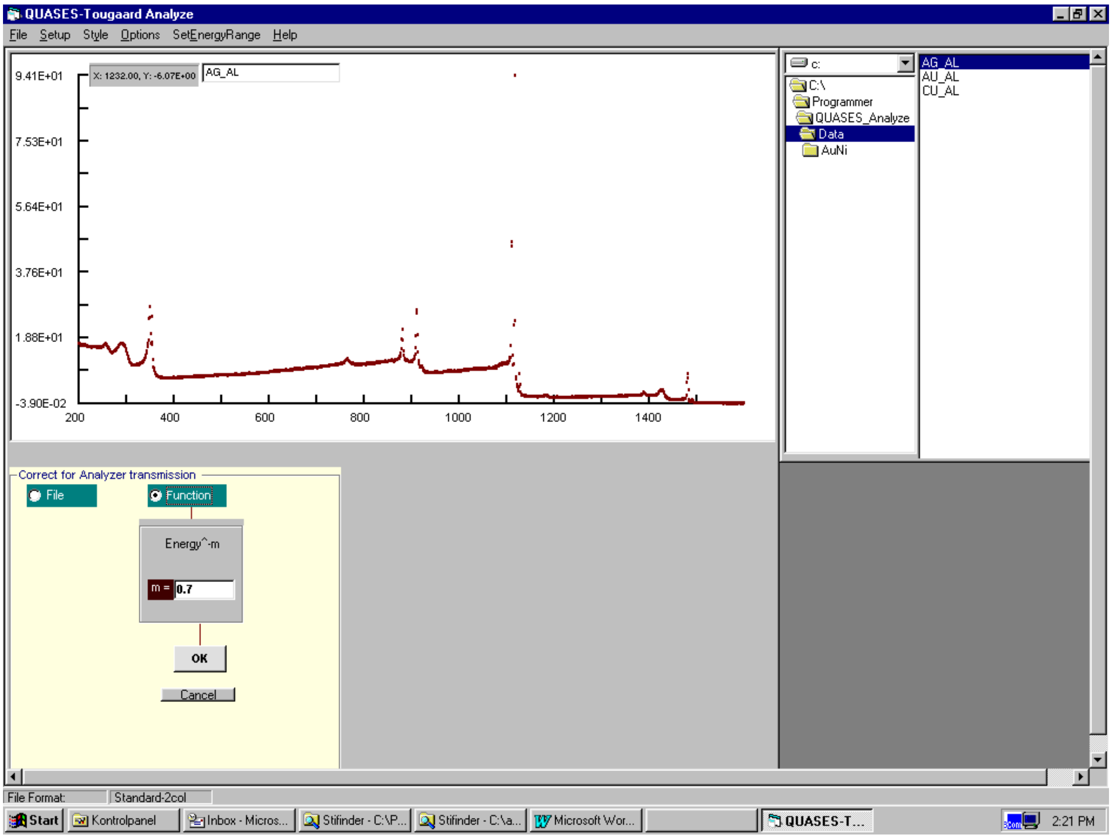


X: 1227.46, Y: -9.17E+00

AG_AL

File Format: Standard-2col

Figure 3.3



X: 1232.00, Y: -6.07E+00

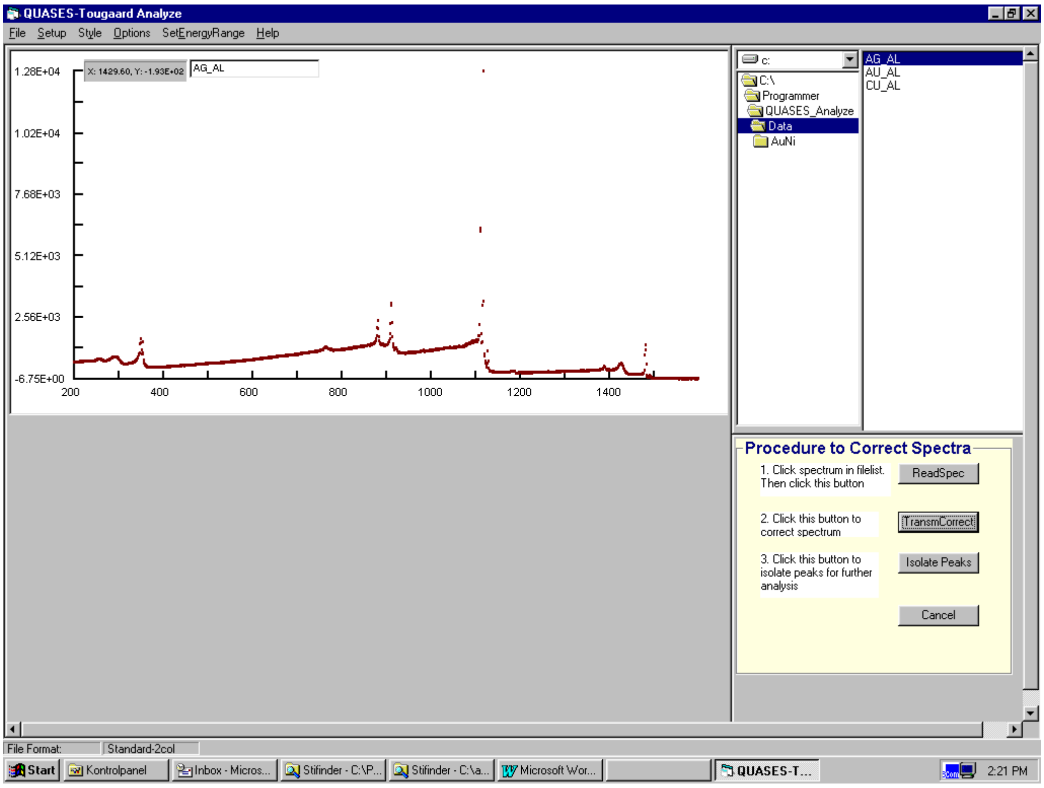
AG_AL

○ File ● Function

m = 0.7

File Format: Standard-2col

Figure 3.4

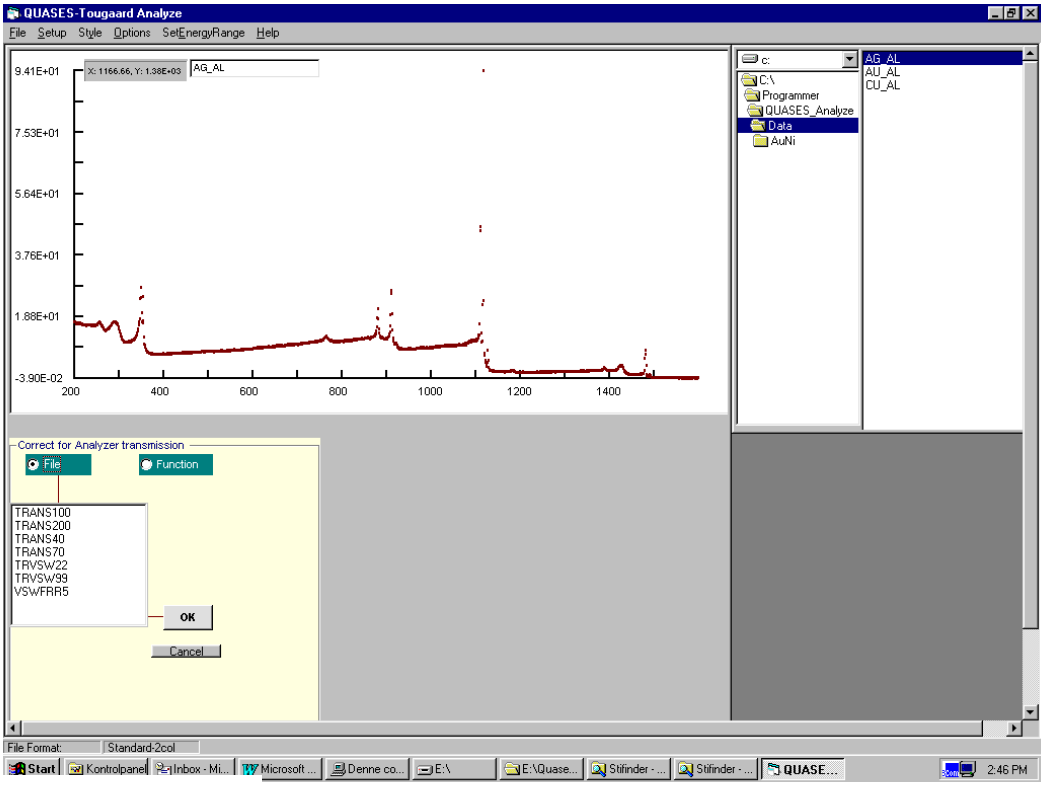


**Procedure to Correct Spectra**

1. Click spectrum in filelist. Then click this button
2. Click this button to correct spectrum
3. Click this button to isolate peaks for further analysis

File Format: Standard-2col

## Figure 3.5



Correct for Analyzer transmission

● File ○ Function

TRANS100
TRANS200
TRANS40
TRANS70
TRVSW22
TRVSW99
VSWFRR5

File Format: Standard-2col

## Figure 3.6

**File**

If the transmission function is stored in a file select the option **File**. Then a list of files is shown (fig.3.6). Select the proper file, which contains the transmission function for the analyzer and click OK. The file with the transmission function must be stored in the **TrsmFct** sub directory. The data format in the file with the transmission function is described in Chapter 6.

## Isolate the Peaks

Now click the **Isolate Peaks** button in fig.3.5 to get fig.3.7. The plotted spectrum has now been corrected for the energy dependence of the analyzer transmission. If a small peak shall be isolated from a spectrum, it is often an advantage to enlarge the peak region. To do this, click **Zoom** then click and hold the left mouse button; drag the mouse to form a box around the peak that you want to isolate, as in fig.3.8. Release the mouse button and get fig.3.9 where the spectrum of the selected region is now plotted.

Click the **Backgr Line** button and get fig.3.10. Position the mouse over either one of the small circles or over the small rectangle. Click and hold the left mouse button and drag the line. In this way, position the line so it matches an energy region on the high energy side of the peak, see fig.3.11. Position the two circles at the lowest and highest energies that you want for the final spectrum.

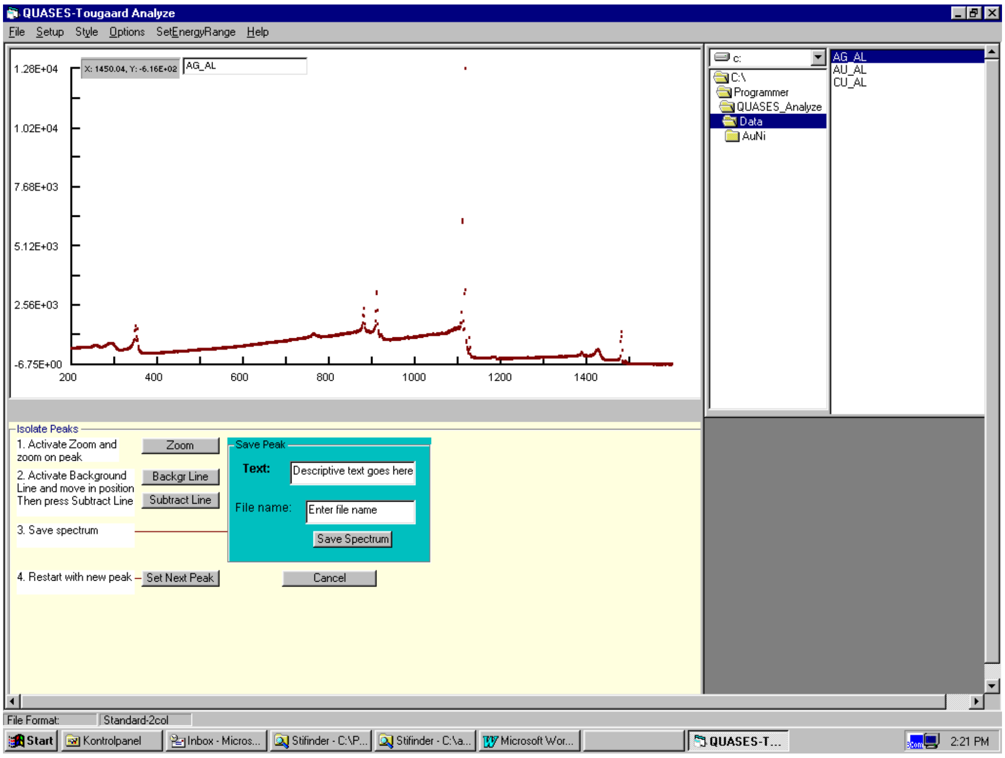
Click **Subtract Line** to subtract the line from the spectrum and get fig.3.12. Note that the energy range of the resulting spectrum has been cut at the low- and high-energy points given by the positions of the circles at the end points of the line that was set in fig.3.11.

Type a descriptive text for the file in the box labeled *Text*: (this text will be stored in the top of the data file). Type a *File name* (here Ag3d). Click **Save Spectrum**. Note that the new file Ag3d now appears in the file list.

To isolate another peak in the spectrum, click **Set Next Peak** and get fig. 3.13.
Click **Zoom** and with the mouse, make a box around another peak (fig.3.13) release the mouse and get fig.3.14. Click **Backgr Line** to get the line on the plot. Move the position and slope of the line with the mouse until it matches the spectrum in an energy region on the high energy side of the peak (fig.3.14). Click **Subtract Line** and get fig.3.15. Type comments in the text box, and a file name (here Ag3p) and then click **Save Spectrum**. Now the spectrum is saved in the data file Ag3p that appears in the file list box (fig.3.15).

This procedure may be repeated to isolate and correct each peak in the spectrum.

Click **Cancel** and get fig.3.16.



Isolate Peaks

1. Activate Zoom and zoom on peak
2. Activate Background Line and move in position Then press Subtract Line
3. Save spectrum
4. Restart with new peak

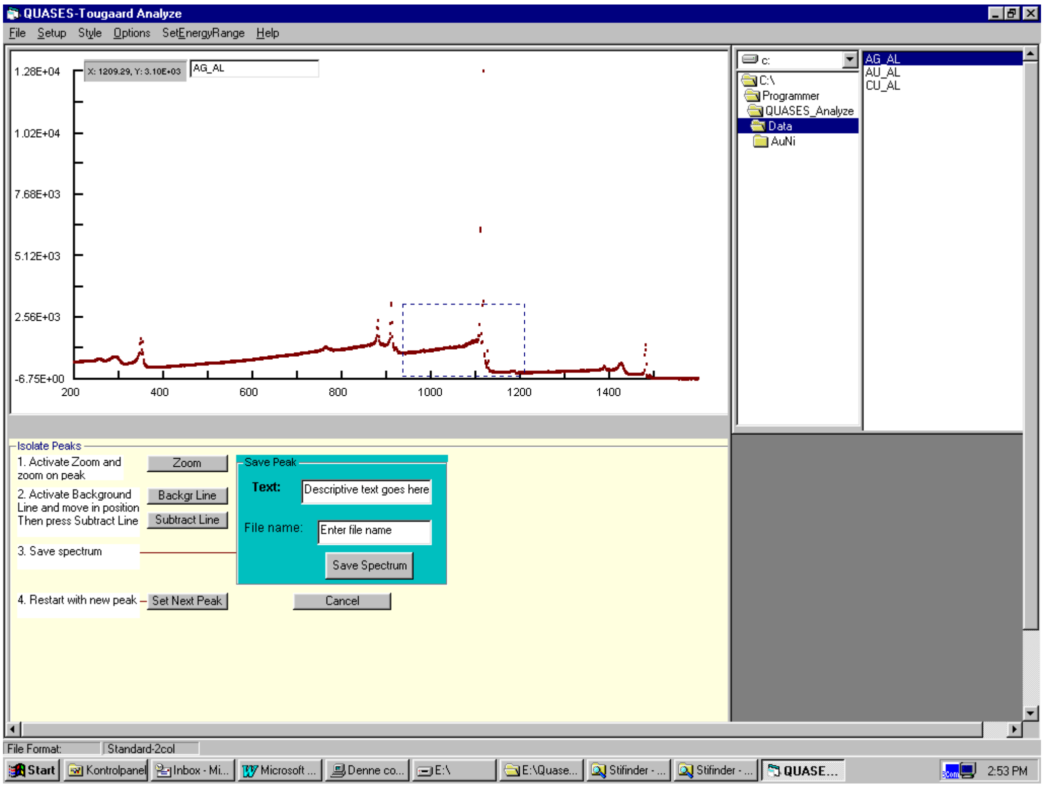
Save Peak

Text: Descriptive text goes here

File name: Enter file name

File Format: Standard-2col

**Figure 3.7**



Isolate Peaks

1. Activate Zoom and zoom on peak
2. Activate Background Line and move in position Then press Subtract Line
3. Save spectrum
4. Restart with new peak

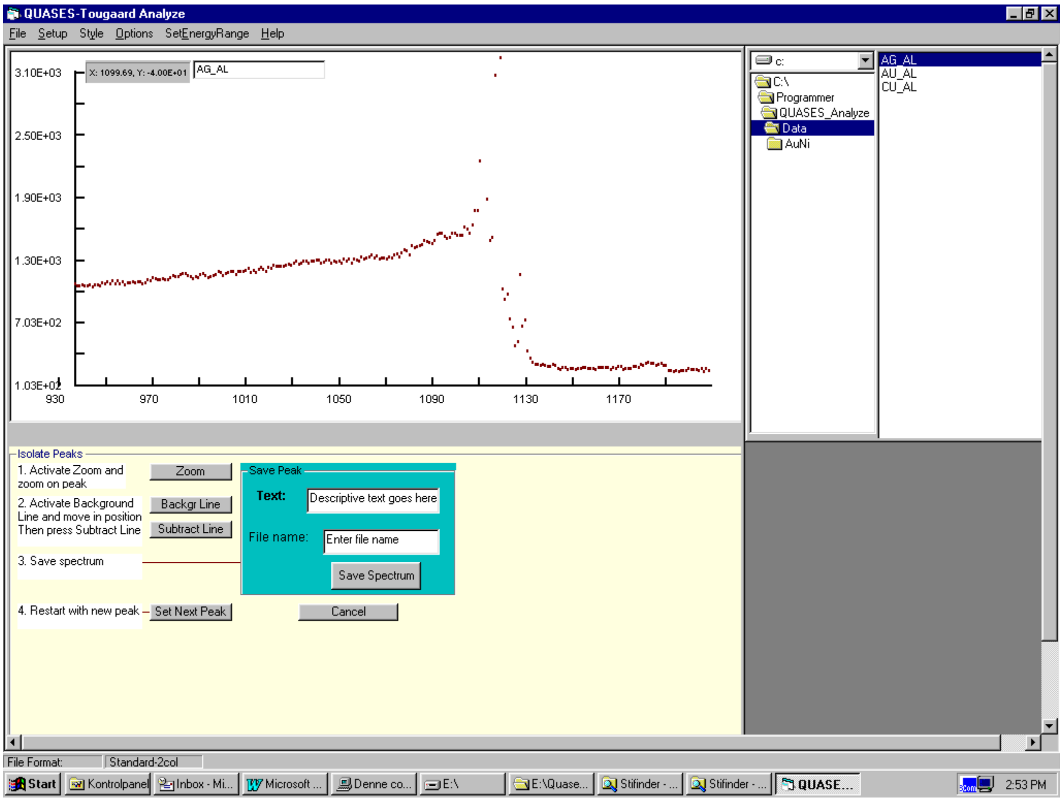
Save Peak

Text: Descriptive text goes here

File name: Enter file name

File Format: Standard-2col

**Figure 3.8**



1. Activate Zoom and zoom on peak

2. Activate Background Line and move in position Then press Subtract Line

3. Save spectrum

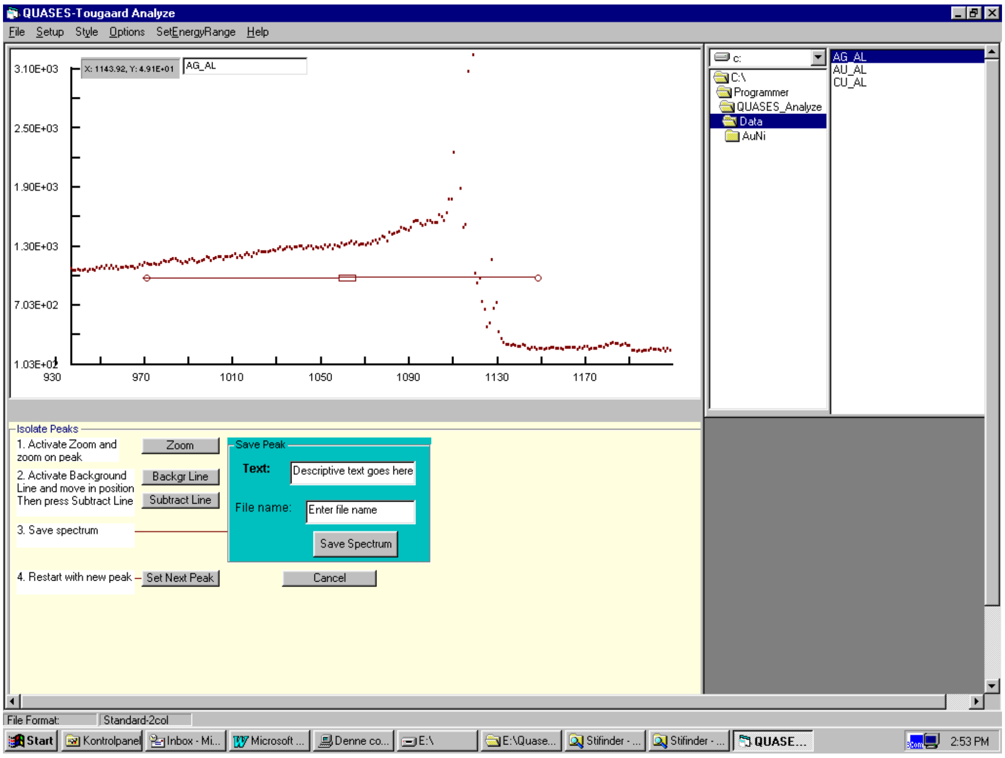
4. Restart with new peak

Text: Descriptive text goes here

File name: Enter file name

File Format: Standard-2col

## Figure 3.9



1. Activate Zoom and zoom on peak

2. Activate Background Line and move in position Then press Subtract Line

3. Save spectrum

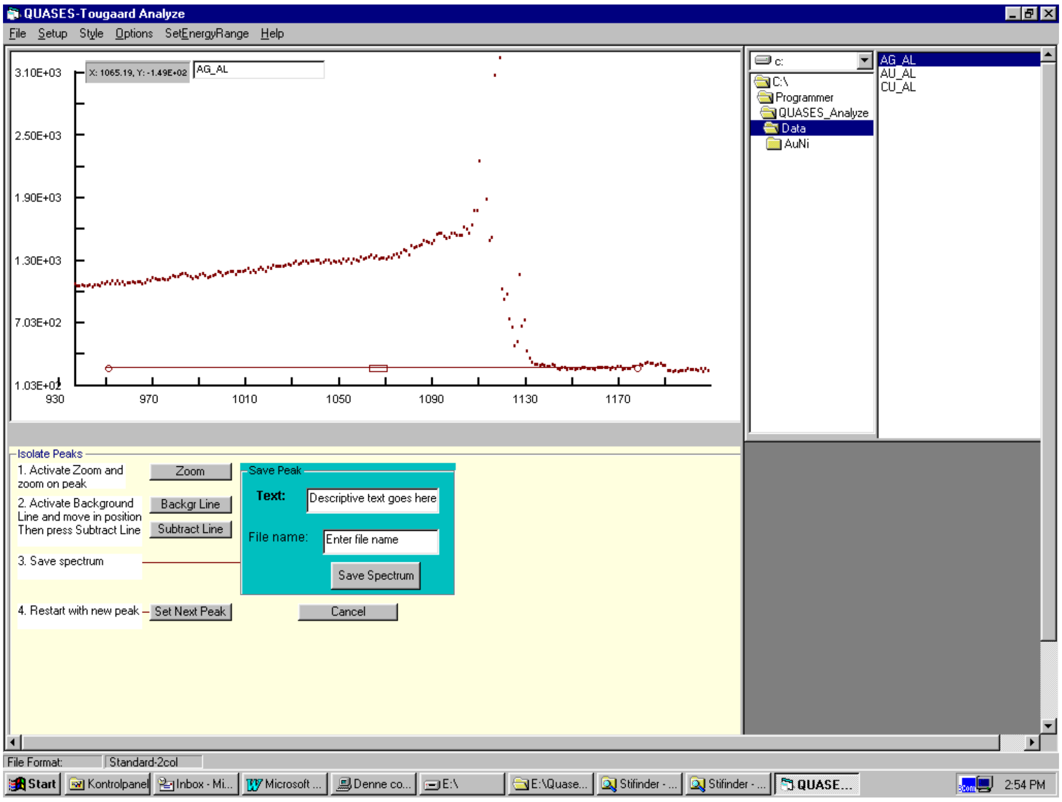
4. Restart with new peak

Text: Descriptive text goes here

File name: Enter file name

File Format: Standard-2col

## Figure 3.10



1. Activate Zoom and zoom on peak

2. Activate Background Line and move in position Then press Subtract Line

3. Save spectrum

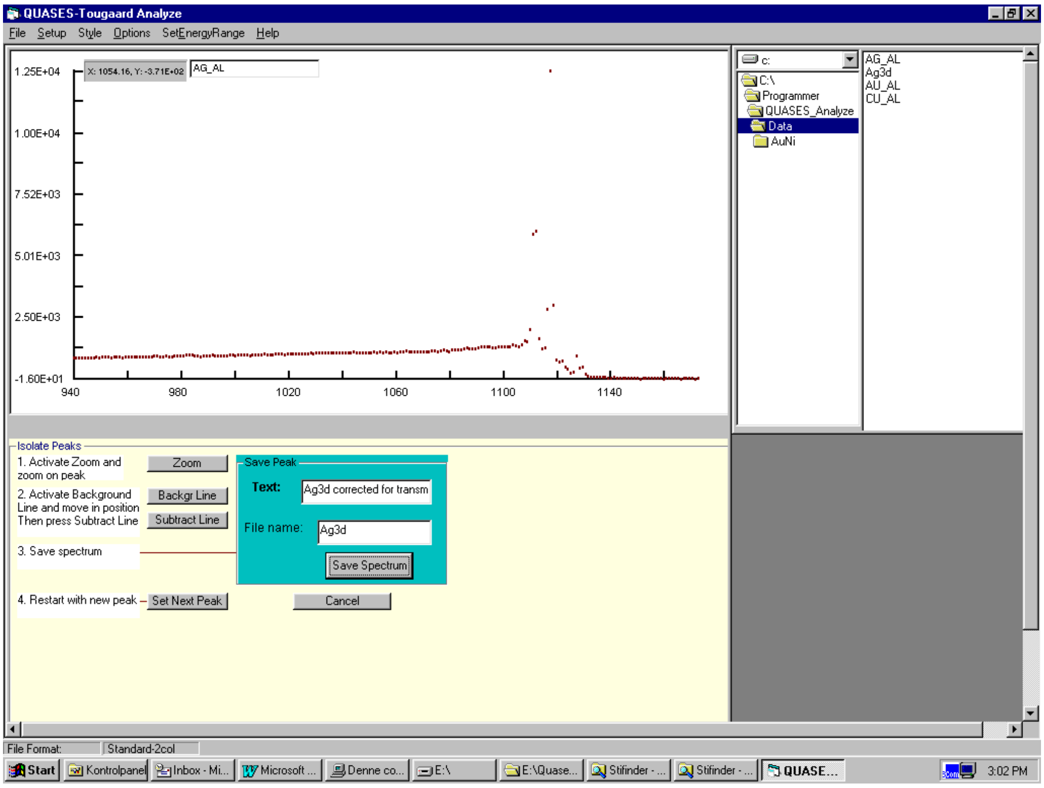
4. Restart with new peak

Text: Descriptive text goes here

File name: Enter file name

File Format: Standard-2col

**Figure 3.11**



1. Activate Zoom and zoom on peak

2. Activate Background Line and move in position Then press Subtract Line

3. Save spectrum

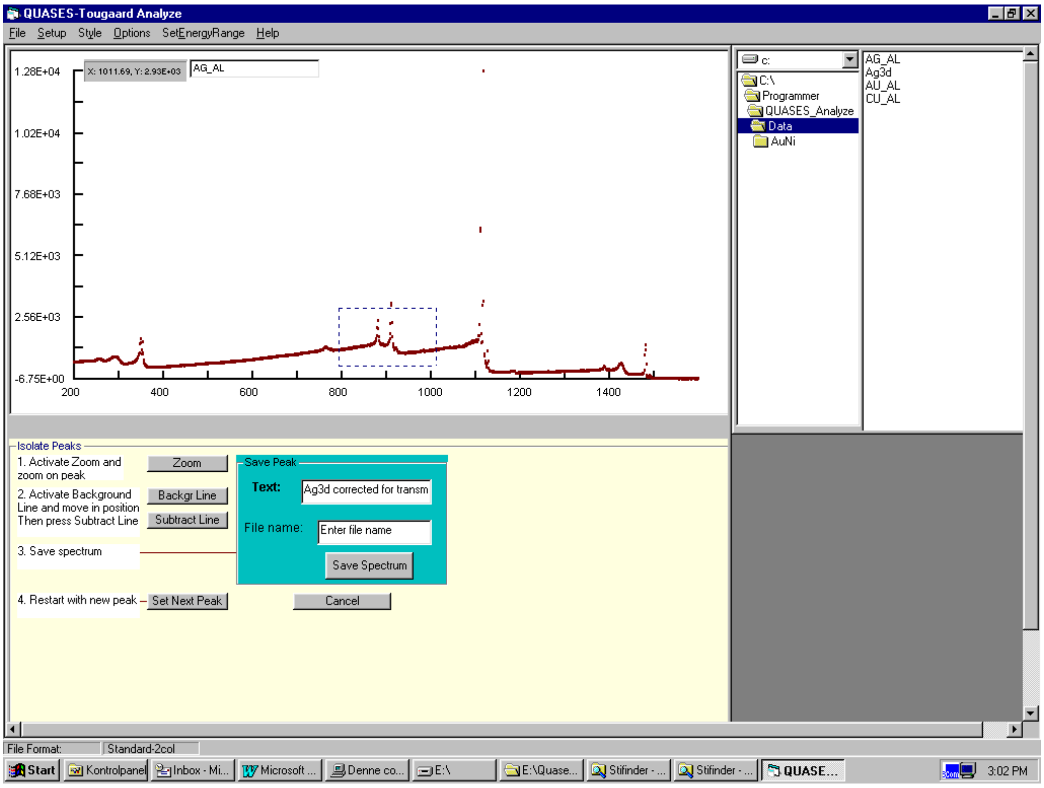
4. Restart with new peak

Text: Ag3d corrected for transm

File name: Ag3d

File Format: Standard-2col

**Figure 3.12**



Isolate Peaks

1. Activate Zoom and zoom on peak
2. Activate Background Line and move in position Then press Subtract Line
3. Save spectrum
4. Restart with new peak

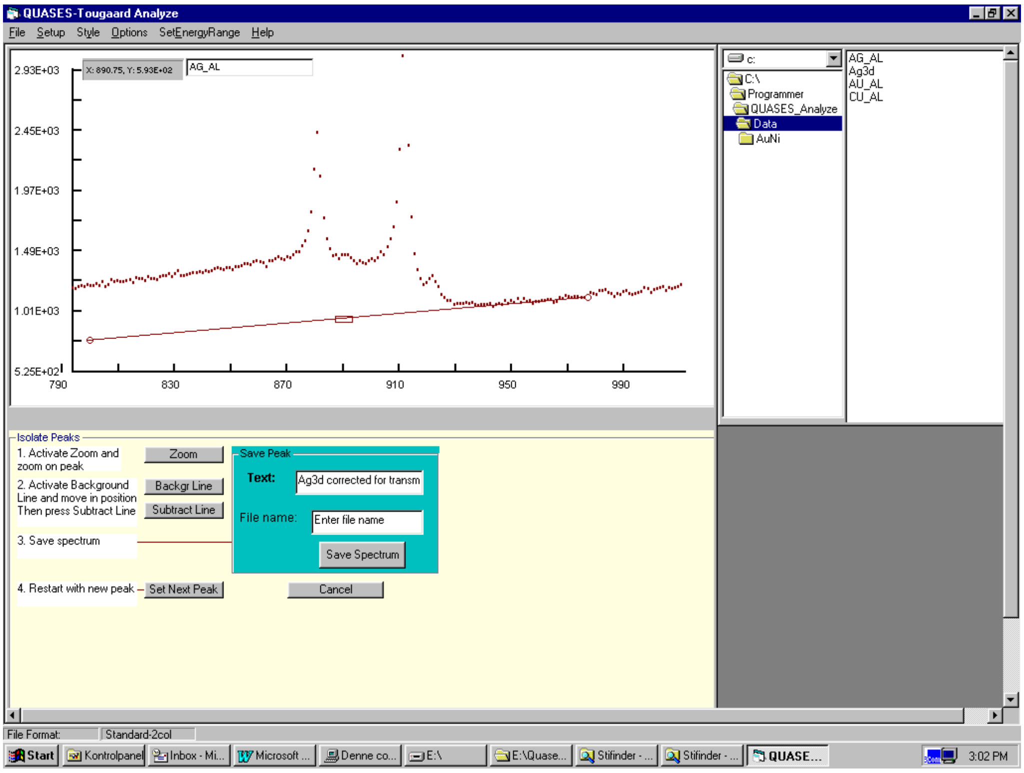
Save Peak

Text: Ag3d corrected for transm

File name: Enter file name

File Format: Standard-2col

Figure 3.13



Isolate Peaks

1. Activate Zoom and zoom on peak
2. Activate Background Line and move in position Then press Subtract Line
3. Save spectrum
4. Restart with new peak

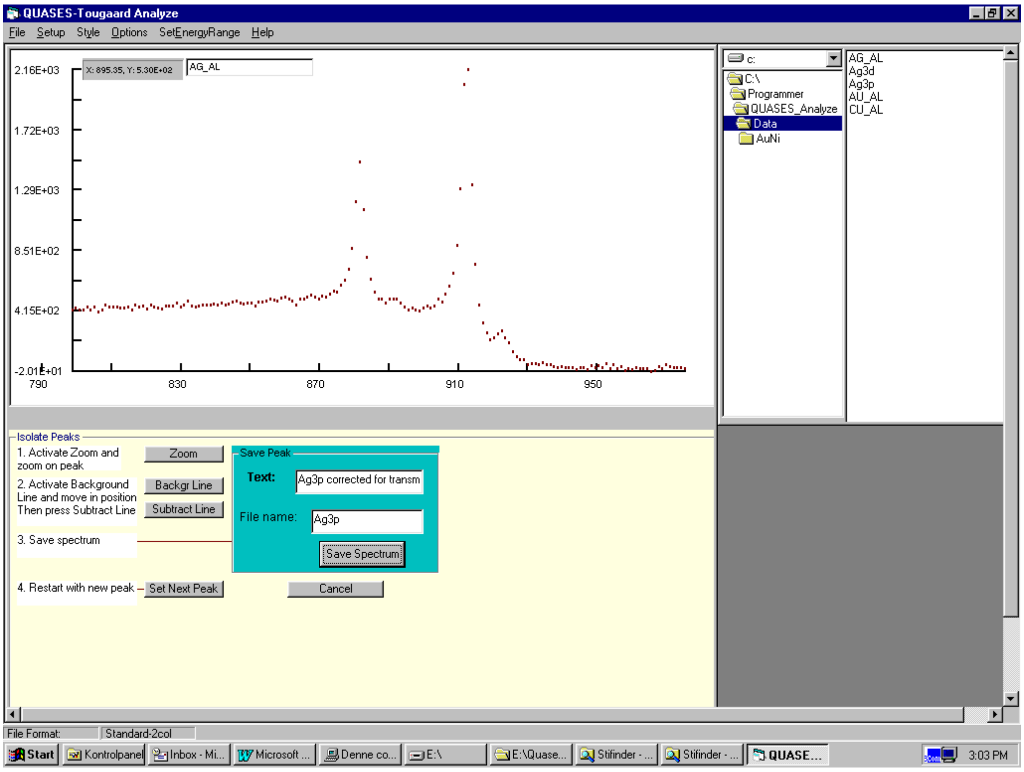
Save Peak

Text: Ag3d corrected for transm

File name: Enter file name

File Format: Standard-2col

Figure 3.14



1. Activate Zoom and zoom on peak

2. Activate Background Line and move in position Then press Subtract Line

3. Save spectrum

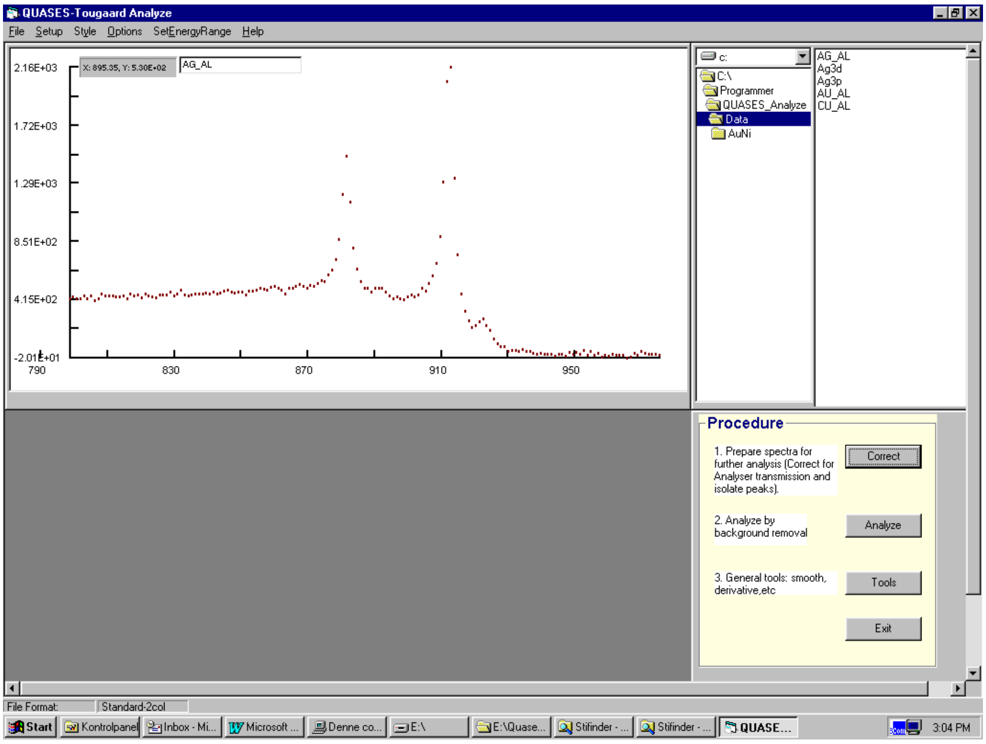
4. Restart with new peak

Text: Ag3p corrected for transm

File name: Ag3p

File Format: Standard-2col

**Figure 3.15**



1. Prepare spectra for further analysis (Correct for Analyser transmission and isolate peaks).

2. Analyze by background removal

3. General tools: smooth, derivative,etc

File Format: Standard-2col

**Figure 3.16**

# *Chapter 4*

# QUASES-Analyze

The purpose of the program **Analyze** is to quantify the composition in the surface region by analysis of the distortion of the peak shape and background signal caused by inelastic scattering of the electrons on their way out of the solid.

The peak shape and background signal depends on the excitation depth for the electrons in the solid (see Chapter 1). The user must therefore give information on the in-depth concentration profile. To facilitate the communication of such information from the user to the program, the depth concentration profiles have been divided into five main classes. Within each class, the user can specify parameters to characterize the details of the in-depth profile.

The five classes of depth concentration profiles are

**Buried Layer**

**Islands (Passive Substrate)**

**Islands (Active Substrate)**

**Exponential Profile**

**Several Buried Layers**

In section 4.1 we describe those parts of the menus that are common to all depth profile classes and the parts that are specific to the individual classes are described in sections 4.2 - 4.6 below.

## 4.1 Menu items common to all depth profile classes

After starting **QUASES-Analyze**, click the box labeled **Analyze** and get fig. 4.1.

Then click **Buried Layer** and get fig. 4.2.

Here follows an explanation of those parameters that are common to all five depth profile classes.

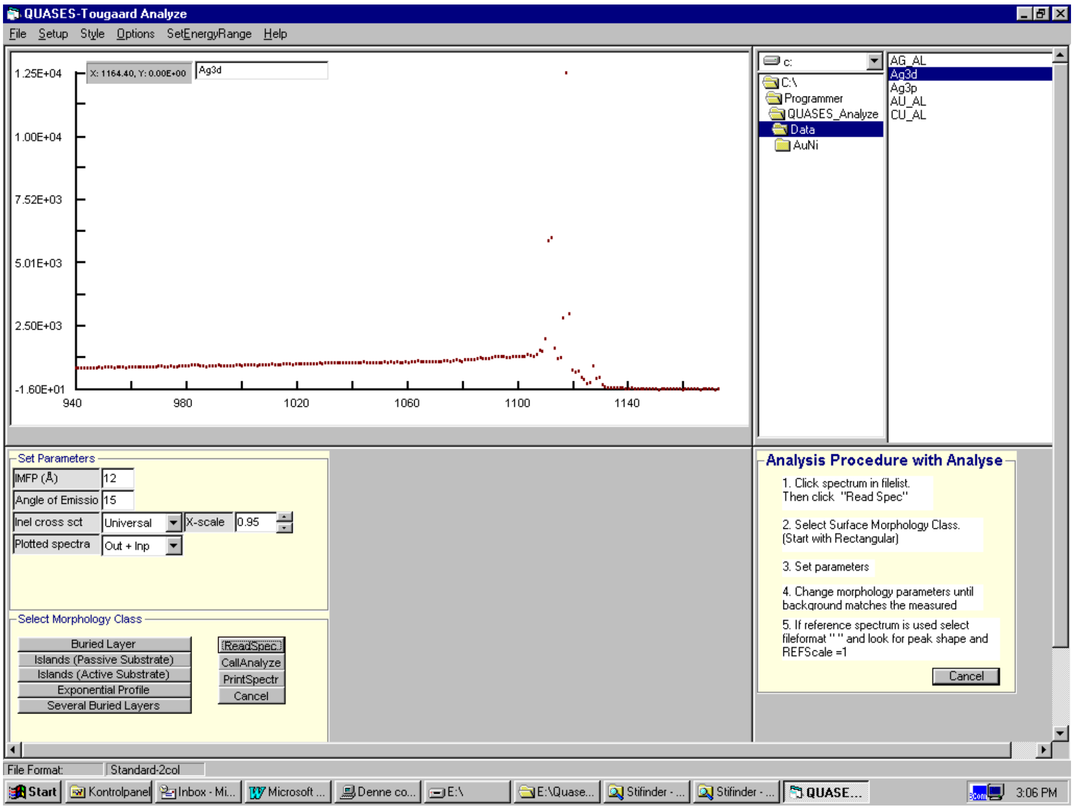
**IMFP (Å)**
This is the inelastic mean free path in Å for the electrons being analyzed. To change the value, click the text box and type the new value.

**Angle of Emission**
This is the angle, in degrees, of electron emission with respect to the surface normal. To change the value, click the text box and type the new value.

**Inelastic cross sct**
This is used to specify the differential cross section for electron energy loss used to calculate the background intensity. Click the arrow next to the text box to display a list of possible cross sections (see fig. 4.3).

> **Universal** (default value) is valid for transition metals and their oxides. This is a good choice in most cases.
>
> **Polymer** should be used when analyzing spectra from polymers
>
> **SiO2** applies to $SiO_2$
>
> **Si** applies to silicon
>
> **Ge** applies to germanium
>
> **Al** applies to aluminum
>
> **File: x-sect** Here the user can specify another cross section (e.g. determined from analysis of a REELS spectrum). This cross section should be saved under the filename x-sect in sub directory X-Sect. The required data format in the file with the cross section is described in Chapter 6.

Select a cross section according to the nature of the solid under investigation by clicking the name of the cross section from the list.
Choose **Universal** if the solid does not fit into any of the listed possibilities.



Set Parameters

IMFP (Å) 12

Angle of Emissio 15

Inel cross sct Universal

X-scale 0.95

Plotted spectra Out + Inp

File Format: Standard-2col

**Analysis Procedure with Analyse**

1. Click spectrum in filelist. Then click "Read Spec"

2. Select Surface Morphology Class. (Start with Rectangular)

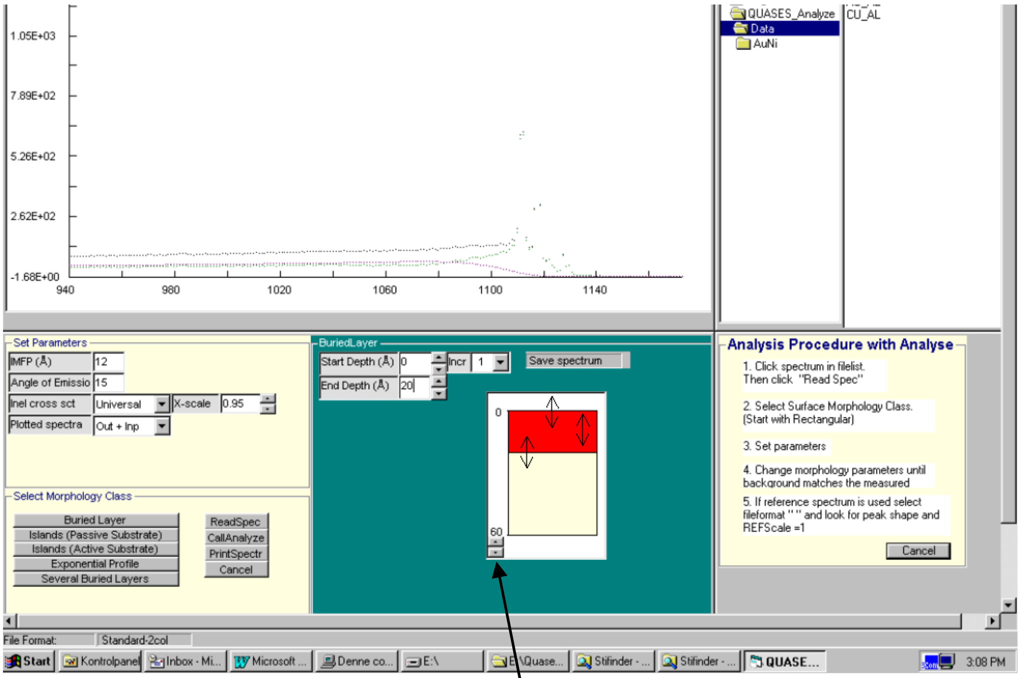
3. Set parameters

4. Change morphology parameters until background matches the measured

5. If reference spectrum is used select fileformat " " and look for peak shape and REFScale =1

Cancel

**Figure 4.1**



Set Parameters

IMFP (Å) 12

Angle of Emissio 15

Inel cross sct Universal

X-scale 0.95

Plotted spectra Out + Inp

Start Depth (Å) 0

Incr 1

End Depth (Å) 20

File Format: Standard-2col

**Analysis Procedure with Analyse**

1. Click spectrum in filelist. Then click "Read Spec"

2. Select Surface Morphology Class. (Start with Rectangular)

3. Set parameters

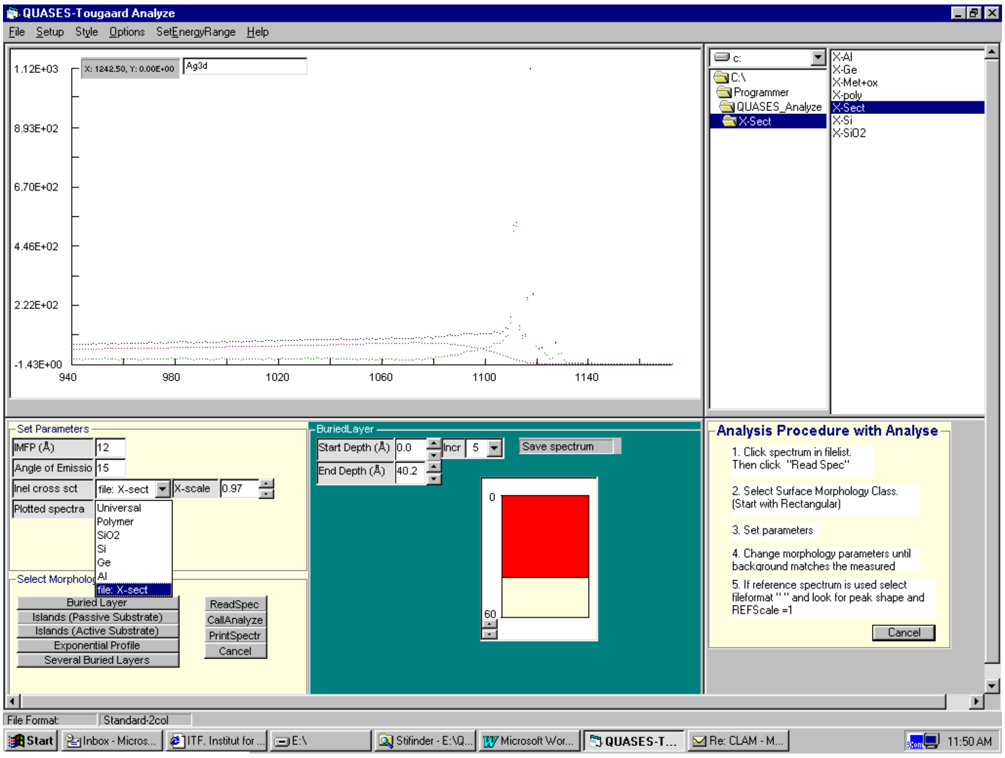
4. Change morphology parameters until background matches the measured

5. If reference spectrum is used select fileformat " " and look for peak shape and REFScale =1

Cancel

**Figure 4.2**

The maximum depth may be changed by clicking the Up-Down arrow.

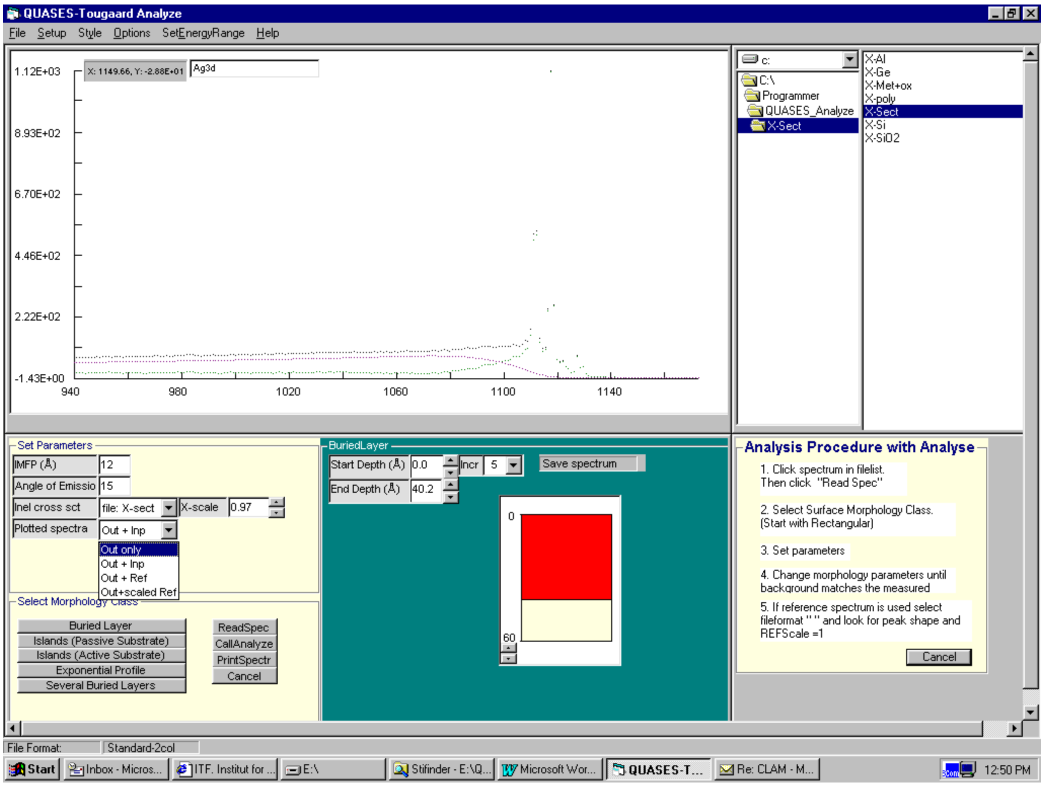


IMFP (Å) 12
Angle of Emissio 15
Inel cross sct file: X-sect
X-scale 0.97
Plotted spectra
Start Depth (Å) 0.0
Incr 5
End Depth (Å) 40.2

**Analysis Procedure with Analyse**

1. Click spectrum in filelist. Then click "Read Spec"
2. Select Surface Morphology Class. (Start with Rectangular)
3. Set parameters
4. Change morphology parameters until background matches the measured
5. If reference spectrum is used select fileformat " " and look for peak shape and REFScale =1

Figure 4.3



IMFP (Å) 12
Angle of Emissio 15
Inel cross sct file: X-sect
X-scale 0.97
Plotted spectra Out + Inp
Start Depth (Å) 0.0
Incr 5
End Depth (Å) 40.2

**Analysis Procedure with Analyse**

1. Click spectrum in filelist. Then click "Read Spec"
2. Select Surface Morphology Class. (Start with Rectangular)
3. Set parameters
4. Change morphology parameters until background matches the measured
5. If reference spectrum is used select fileformat " " and look for peak shape and REFScale =1

Figure 4.4

**X-scale**
This is used to scale the magnitude of the cross section for inelastic electron scattering by the factor given in the textbox. Use 0.95 unless other information on the value is available. The value may be changed by clicking the Up-Down arrows next to the textbox or by clicking within the textbox and type a new value.

**Plotted spectra** is used to specify the format of the output on the screen.
The user can select between 4 options (see fig.4.4):

> **Out only**, to display only the background corrected output spectrum.
>
> **Out + Inp (default value)**, to display the background corrected output spectrum, the input spectrum, and the background spectrum.
>
> **Out+Ref**, to display the background corrected output spectrum, the reference spectrum, and the difference between the output and the reference spectra. This is a helpful option when an atomic reference spectrum is known. The profile may then be varied until a good match with the reference is obtained. However the user will in most cases prefer to use the **Out+scaled Ref** option below.
>
> **Out+scaled Ref**, to display the background corrected output spectrum, the reference spectrum with the intensity scaled, and the difference between the output and the reference spectra. This option is used when a reference spectrum is available. In comparison to **Out+Ref** it is easier to compare the spectral shapes of the background corrected and the reference because the reference spectrum is scaled to the same intensity as the background corrected. The scaling factor is calculated to give the same area in the energy range between two energy lines (see below) of the scaled reference spectrum as the area of the spectrum after analysis. The scaling factor will be shown in a textbox on the screen. The concentration depth profile of the atoms corresponding to the measured peak has been determined when **ScalingFactor** = 1, and the shape of the background analyzed roughly matches the reference spectrum.

If the output format **Out+Ref** or **Out+ scaled Ref** were selected, the textbox **Ref spct** is shown (see fig. 4.5). Here the user must give the name of the file with the reference spectrum. To do this,

- Click OK
- In the *filelist*, click the filename that holds the data of the reference spectrum. This spectrum is plotted together with the analyzed and the filename appears in the text box.

To change to another reference spectrum,

- Click the textbox to the right of **Ref spct**.
- Click OK

- In the *filelist*, click the filename that holds the data of the reference spectrum.

If there is an energy shift between the reference spectrum and the analyzed spectrum, this can be corrected for by changing the value of **Eshift** (see fig.4.5). **Eshift** may be changed either by clicking within the textbox and typing the new value or by using the Up-Down arrows next to the **Eshift** textbox.

If **Output format Out+scaled Ref** was selected, two vertical lines appear in the plot (see fig. 4.5). The position of these lines may be changed with the mouse by positioning the mouse icon over one of the lines, then click and hold the left mouse button and drag the line to the new position.

Three new textboxes also appear in the **Set Parameters window**:

**E1** shows the energy position of the left line

**E2** shows the energy position of the right line

**Ap** shows the peak area of the background-corrected spectrum in the energy region from E1 to E2.

The energy range from **E1** to **E2** is also used to calculate the scaling factor multiplied on the reference spectrum.

In the **Buried Layer window**, three new textboxes appear (fig.4.6).

**Scalefactor** shows the value of the calculated scaling factor, which is the ratio of peak areas between **E1** and **E2**

$$Scalefactor = \frac{\sum x(i) \cdot \Delta E}{\sum z(i) \cdot \Delta E_{ref}}$$

where x(i) is the background corrected spectrum and z(i) the reference spectrum.
The plotted reference spectrum has been multiplied by this *Scalefactor*.

**RMS deviat** shows the root mean square deviation between the calculated background corrected spectrum and the scaled reference spectrum calculated in the energy range from **E1** to **E2** according to:

$$RMS = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x(i) - Scalefactor * z(i))^2}$$

where N is the number of data points in the energy range from **E1** to **E2** and x(i) and z(i) are the background corrected spectrum and the reference spectrum.

**Optimize RMS.** When this button is clicked the **Start Depth** and **End Depth** are varied automatically over a certain range, and a minimum in RMS is identified. The new start and end depths are displayed and the plot is updated.

**Optimize Area**. When this button is clicked the **Start Depth** and **End Depth** are varied automatically over a certain range, and the value as close as possible to Scalefactor = 1.00 is identified. The new start and end depths are displayed and the plot is updated.

**Print the spectra.**

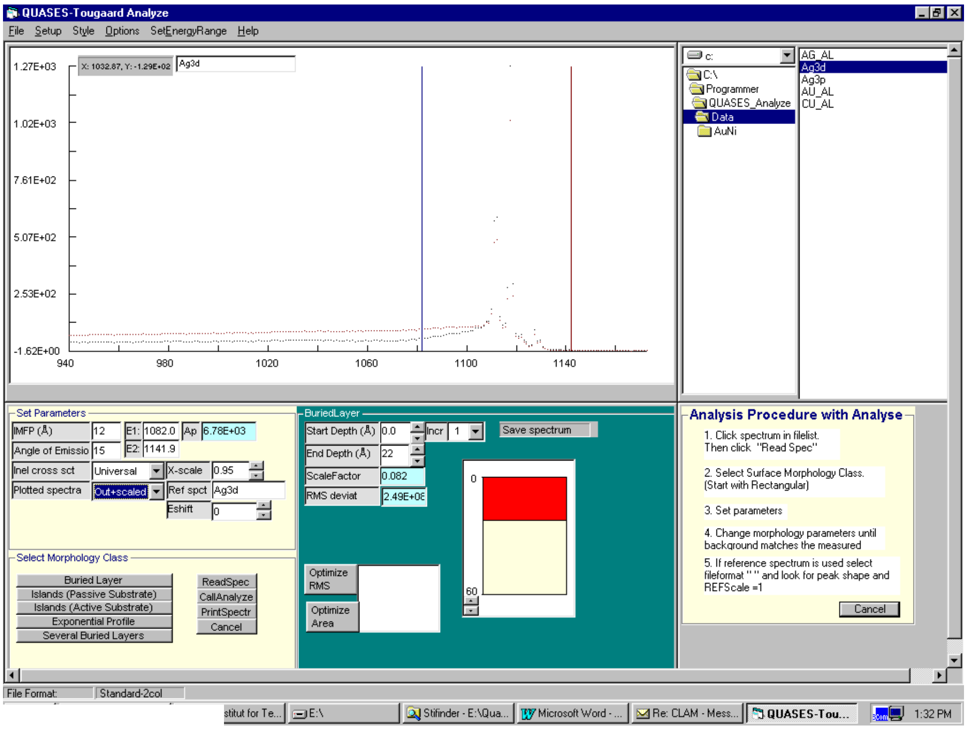
To print the spectra displayed on the plot screen, click the **PrintSpectr** button.

**Save spectrum**

To save the background corrected spectrum click **Save Spectrum** and get fig.4.6.

Type any comments that you may wish to store with the spectrum and select a filename.

Click **Save spectrum**. The new file appears in the filelist box.



Set Parameters

IMFP (Å): 12
E1: 1082.0
Ap: 6.78E+03
Angle of Emissio: 15
E2: 1141.9
Inel cross sct: Universal
X-scale: 0.95
Plotted spectra: Out+scaled
Ref spct: Ag3d
Eshift: 0

BuriedLayer

Start Depth (Å): 0.0
Incr: 1
End Depth (Å): 22
ScaleFactor: 0.082
RMS deviat: 2.49E+08

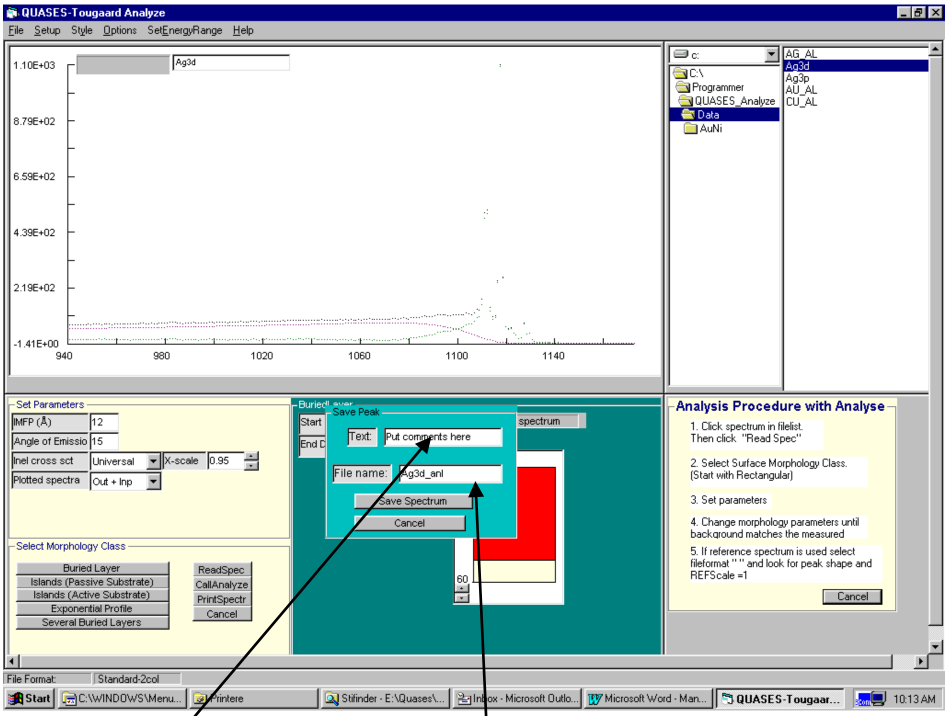
Select Morphology Class

**Analysis Procedure with Analyse**

1. Click spectrum in filelist.
Then click "Read Spec"
2. Select Surface Morphology Class.
(Start with Rectangular)
3. Set parameters
4. Change morphology parameters until background matches the measured
5. If reference spectrum is used select fileformat " " and look for peak shape and REFScale =1

File Format: Standard-2col

**Figure 4.5**



Set Parameters

IMFP (Å): 12
Angle of Emissio: 15
Inel cross sct: Universal
X-scale: 0.95
Plotted spectra: Out + Inp

Select Morphology Class

BuriedLayer

Save Peak

Text: Put comments here
File name: Ag3d_anl

**Analysis Procedure with Analyse**

1. Click spectrum in filelist.
Then click "Read Spec"
2. Select Surface Morphology Class.
(Start with Rectangular)
3. Set parameters
4. Change morphology parameters until background matches the measured
5. If reference spectrum is used select fileformat " " and look for peak shape and REFScale =1

File Format: Standard-2col

**Figure 4.6**

Type the filename. Default name is the name of the spectrum followed by _anl

Type comments. These will be stored in the top of the data file.

## 4.2 Buried Layer

This is used to analyze the peak shape and background from rectangular in-depth concentration profiles.

The upper and lower bounds of the rectangular profile can be chosen arbitrarily. This class of profiles can therefore be used to model a wide variety of solids including substrates with an overlayer, an overlayer on a substrate, a buried layer, and a homogeneous solid. This profile is therefore usually be the first attempt when analyzing a spectrum.

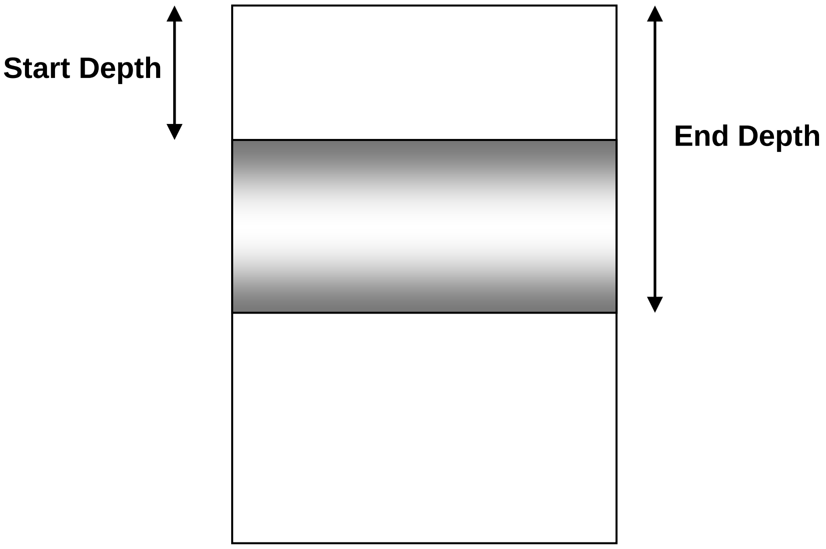


Figure 4.7

Click the **Analyze** box.

In the filelist, click the filename (here Au_ref) with the XPS-spectrum.

Click **ReadSpec** and get fig.4.1.

Click **Buried Layer** and get fig.4.2.

In the **Buried Layer – window** the

**Start Depth** is the depth in Å where the buried layer starts

**End Depth** is the depth in Å where the buried layer ends (fig. 4.7).

The **inset picture** gives a visualization of the surface structure.

The maximum depth plotted in the inset picture may be changed by clicking the Up-Down arrow in the lower left part of the **inset picture.**(see fig.4.2).

There are three ways to change the in-depth concentration profile.

Either

- Click the text box and type the new **Start Depth** or **End Depth**.

or

- Click the Up-Down arrows next to the text boxes. The increments each time the arrows are clicked is given by the value in the textbox **Incr**. The Increment may be changed by clicking the arrow next to the **Incr** textbox (see fig.4.9) and select a new value from the list.

or

- Move the mouse over the region of the Start or End depth in the inset picture. The mouse icon changes to an arrow (see fig.4.2). Now click the left mouse button, hold the button and drag the mouse icon to the new desired depth and finally release the mouse button.

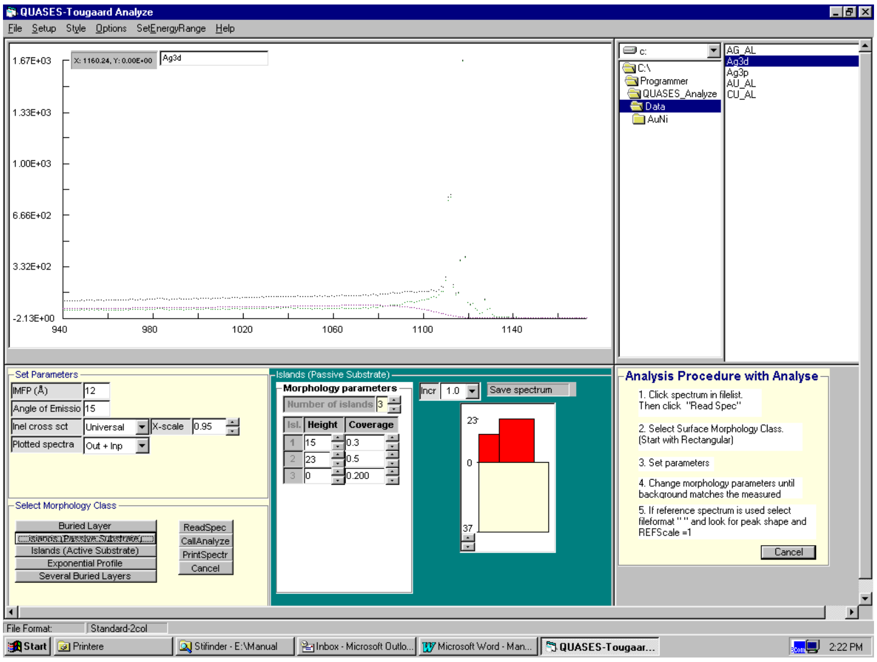
or

- Move the mouse over the center depth of the rectangular profile. The mouse icon changes to an arrow (see fig.4.2). Now click the left mouse button, hold the button and drag the mouse icon to the new desired depth and finally release the mouse button.

The background correction to the spectrum is calculated from the morphology specified in the **Buried Layer window** and the parameters that are set in the **Set Parameter window**.

Whenever a parameter is changed, the calculation is updated and the new background correction is plotted.

In the plot now appear three spectra. The original spectrum, the spectrum corrected for the background and the background.



X: 1160.24, Y: 0.00E+00

Ag3d

Set Parameters

IMFP (Å): 12

Angle of Emissio: 15

Inel cross sct: Universal

X-scale: 0.95

Plotted spectra: Out + Inp

Islands (Passive Substrate)

Morphology parameters

Number of islands: 3

Incr: 1.0

| Isl. | Height | Coverage |
|---|---|---|
| 1 | 15 | 0.3 |
| 2 | 23 | 0.5 |
| 3 | 0 | 0.200 |

Analysis Procedure with Analyse

1. Click spectrum in filelist.
Then click "Read Spec"

2. Select Surface Morphology Class.
(Start with Rectangular)

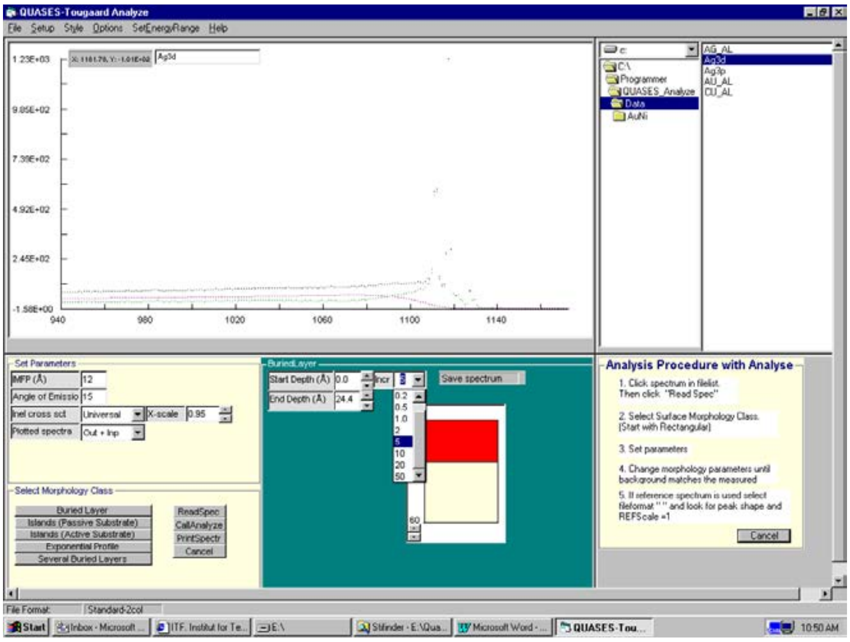
3. Set parameters

4. Change morphology parameters until background matches the measured

5. If reference spectrum is used select fileformat " " and look for peak shape and REFScale =1

File Format: Standard-2col

Figure 4.9



Ag3d

Set Parameters

IMFP (Å): 12

Angle of Emissio: 15

Inel cross sct: Universal

X-scale: 0.95

Plotted spectra: Out + Inp

BuriedLayer

Start Depth (Å): 0.0

End Depth (Å): 24.4

Incr: 5

Analysis Procedure with Analyse

1. Click spectrum in filelist.
Then click "Read Spec"

2. Select Surface Morphology Class.
(Start with Rectangular)

3. Set parameters

4. Change morphology parameters until background matches the measured

5. If reference spectrum is used select fileformat " " and look for peak shape and REFScale =1

File Format: Standard-2col

Figure 4.10

## 4.3 Islands (Passive Substrate)

This is used to analyze the peak shape and background from islands (see fig. 4.8). **Island (Passive Substrate)** treats the spectrum of electrons emitted from the overlayer atoms. Another option **Islands (Active Substrate)** treats the spectrum of electrons emitted from the substrate atoms of a similar structure (see Section 4.4 below).

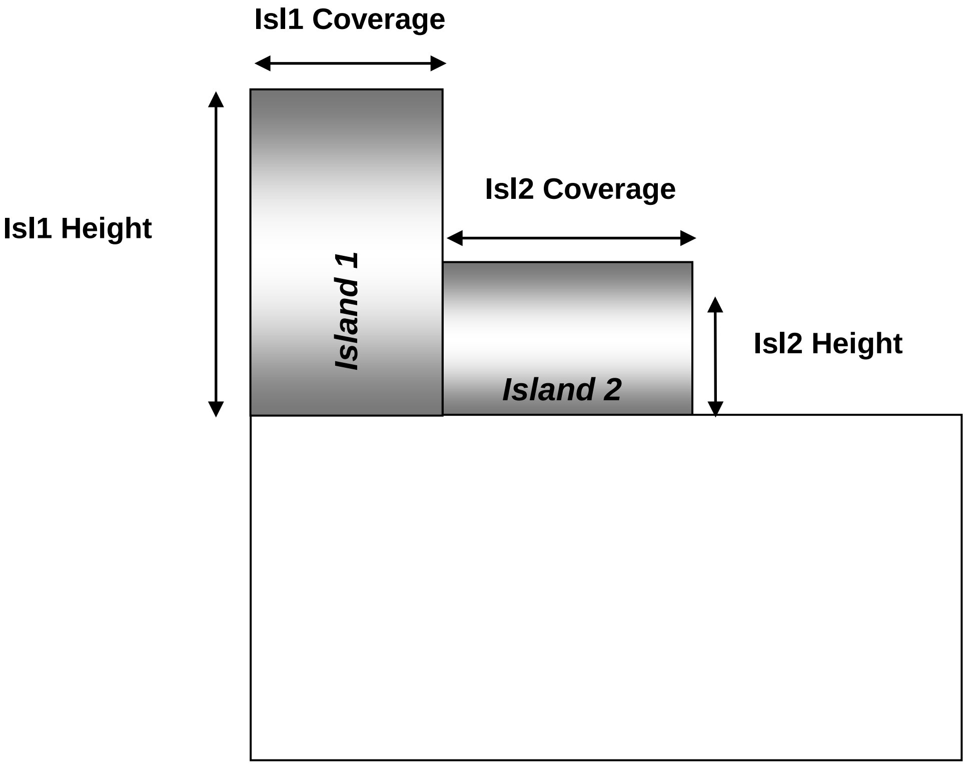


**Figure 4.8.** The number of islands their heights and coverage define the structure.

Click the box labeled **Analyze**.
In the filelist, click the filename (here Ag3d) with the XPS-spectrum.
Click **ReadSpec**.

Click **Islands (Passive Substrate)** and get fig.4.10.

In the **Islands (Passive Substrate) – window** parameters can be set.

**Number of islands** this number can be changed by clicking the Up-Down arrow.

**Height** is the height in Å of each island

**Coverage** is the fraction of the surface covered by this island

The **inset picture** gives a visualization of the surface structure.

The maximum depth plotted in the inset picture may be changed by clicking the Up-Down arrow (see fig.4.2).

If the selected total coverage exceeds 1, the program recalculates the coverage of the last island to fulfill the constraint that the total coverage cannot exceed 1.

To model a structure with islands that cover a total of less than 1, set the height of the last island to zero.

The island structure can be changed by

Changing the **Number of islands**. The maximum number of islands is 9.

Changing the **Height** and **Coverage** of each island
To do this,

either

Click the text box and type the new **Height** and **Coverage**.

or

Click the Up-Down arrows next to the text boxes. The height changes each time the arrows are clicked by the value in the textbox **Incr**. The Increment may be changed by clicking the arrow next to the **Incr** textbox (see fig.4.9) and select a new value from the list. The coverage changes by 0.05 for each mouse click.

(Note: the morphology can not be changed by dragging the mouse icon over the picture as in the case of a Buried Layer)

## 4.4 Islands (Active Substrate)

This is used to analyze the peak shape and background from a structure of islands. **Island (Active Substrate)** is used to analyze the spectrum of electrons emitted from the substrate atoms after they have passed through the overlayer islands (see fig. 4.11). Another option **Island (Passive Substrate)** treats the spectrum of electrons emitted from the overlayer atoms of a similar island structure (see Section 4.3).

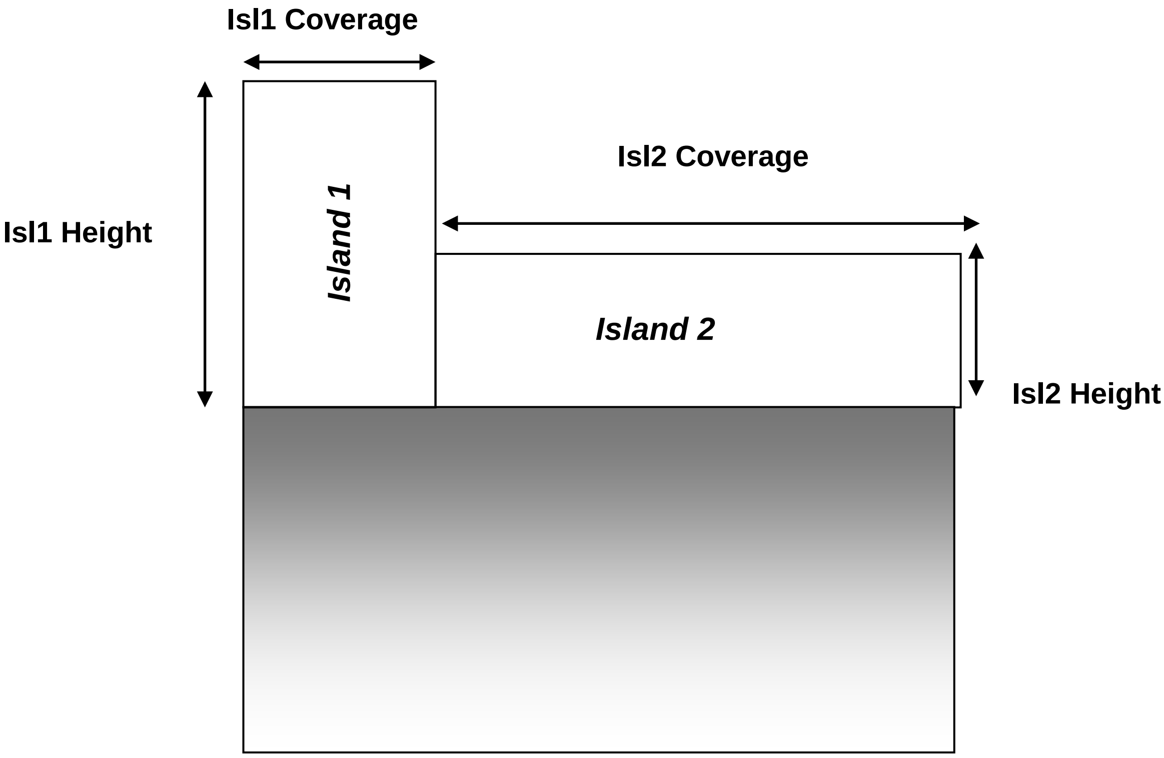


**Figure 4.11** The height and coverage of the two islands.

Click the **Analyze** box.
In the filelist, click the filename (here Ag3d) with the XPS-spectrum.
Click **ReadSpec.**

Click **Islands (Active Substrate)** and get fig.4.12.

In the **Islands (Active Substrate) – window** the

**Height** is the height in Å of each of the two islands.

**Coverage** is the fraction of the surface covered by this island

The **inset picture** gives a visualization of the surface structure.

The maximum depth plotted in the inset picture may be changed by clicking the Up-Down arrow (see fig.4.2).

To model the effect of a single island, set the height of island 2 to zero.

**Note that the number of islands is limited to two. This can not be changed.**

The structure can be changed by

Changing the **Height** and **Coverage** of each island
To do this,

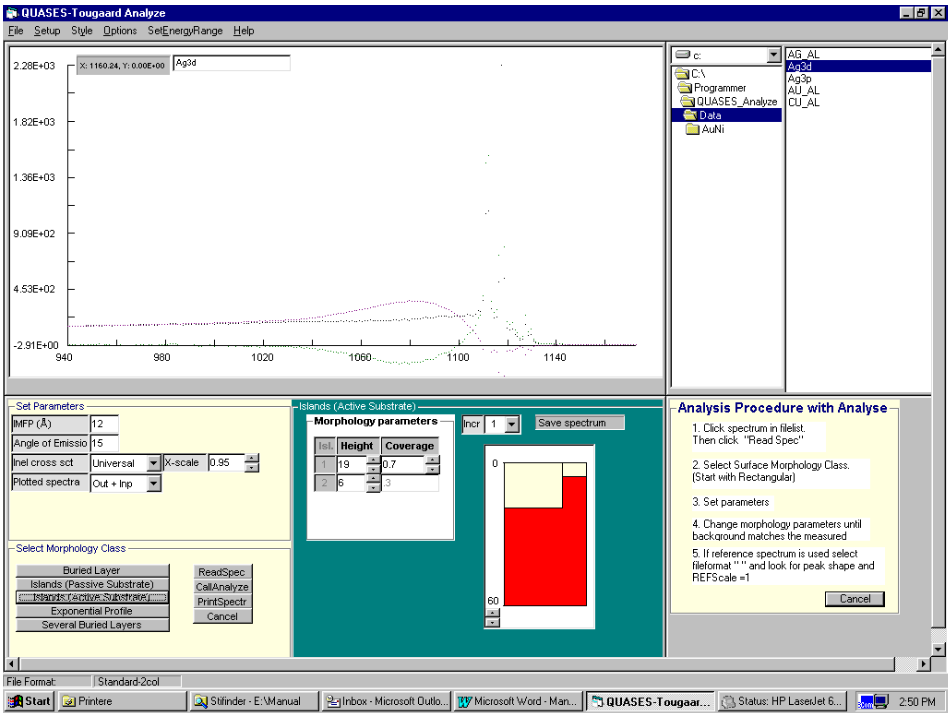
either

Click the text box and type the new **Height** and **Coverage**.

or

Click the Up-Down arrow next to the text boxes. The height changes each time the arrows are clicked by the amount in the textbox **Incr**. The increment may be changed by clicking the arrow next to the **Incr** textbox (see fig.4.9) and select a new value from the list. The coverage changes by 0.05 for each mouse click.

(Note: the morphology can not be changed by dragging the mouse icon over the picture as in the case of a Buried Layer)



IMFP (Å) 12
Angle of Emissio 15
Inel cross sct Universal
X-scale 0.95
Plotted spectra Out + Inp

Incr 1

| Isl. | Height | Coverage |
|---|---|---|
| 1 | 19 | 0.7 |
| 2 | 6 | .3 |

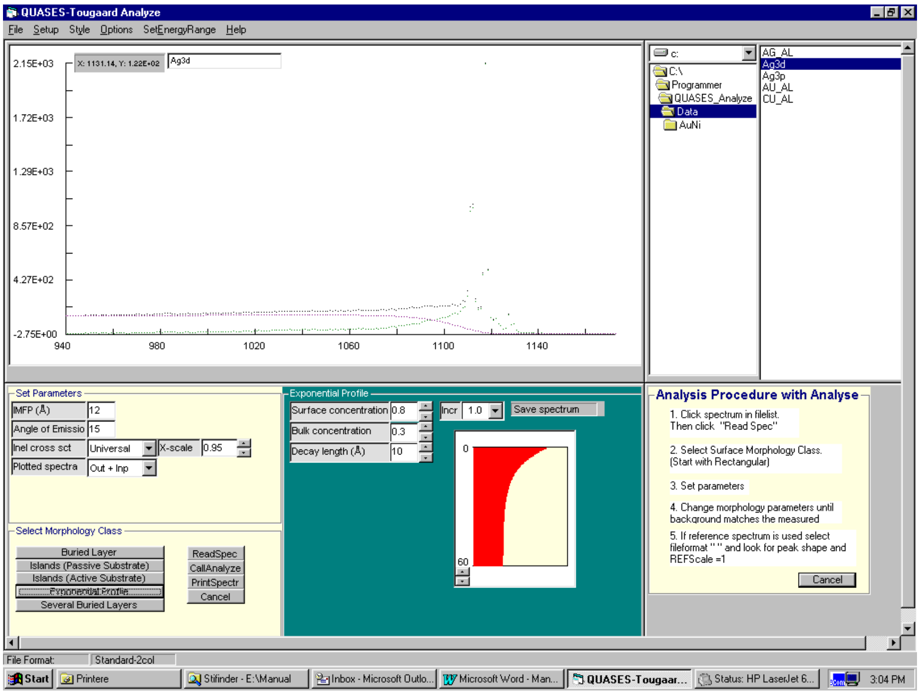
File Format: Standard-2col

**Analysis Procedure with Analyse**

1. Click spectrum in filelist.
Then click "Read Spec"
2. Select Surface Morphology Class.
(Start with Rectangular)
3. Set parameters
4. Change morphology parameters until background matches the measured
5. If reference spectrum is used select fileformat " " and look for peak shape and REFScale =1

Cancel

Figure 4.12



IMFP (Å) 12
Angle of Emissio 15
Inel cross sct Universal
X-scale 0.95
Plotted spectra Out + Inp

Surface concentration 0.8
Bulk concentration 0.3
Decay length (Å) 10
Incr 1.0

File Format: Standard-2col

**Analysis Procedure with Analyse**

1. Click spectrum in filelist.
Then click "Read Spec"
2. Select Surface Morphology Class.
(Start with Rectangular)
3. Set parameters
4. Change morphology parameters until background matches the measured
5. If reference spectrum is used select fileformat " " and look for peak shape and REFScale =1

Cancel

Figure 4.13

## 4.5 Exponential Profile.

This is used to analyze the peak shape and background from exponential in-depth concentration profiles (see fig. 4.14). The profile may be either exponentially increasing or decreasing with depth and the surface and the bulk concentrations may have any value between 0 and 1.

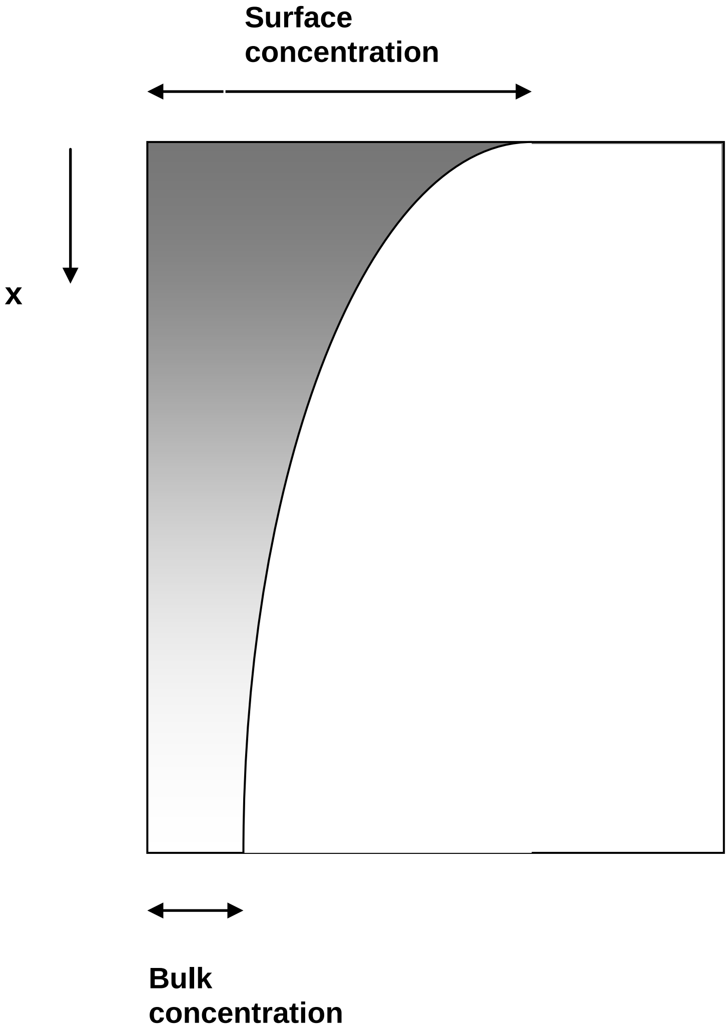


**Figure 4.14** The exponential in-depth concentration profile.

Click the box labeled **Analyze**.

In the filelist, click the filename (e.g. Ag3d) with the XPS-data.

Click **ReadSpec**.

Click **Exponential Profile** and get fig.4.13.

In the **Exponential Profile – window** the

> **Surface concentration** is the concentration at the surface (value between 0 and 1. If the input is outside of this range, the program selects the nearest allowed value).
>
> **Bulk concentration** is the concentration deep in the bulk (value between 0 and 1. If the input is outside of this range, the program selects the nearest allowed value).
>
> **Decay length** is the decay length in Å of the exponential profile.
>
> The **inset picture** gives a visualization of the surface structure.
>
> The maximum depth plotted in the inset picture may be changed by clicking the Up-Down arrow (see fig.4.2).

The concentration profile is thus

$$f(x) = C_B + (C_S - C_B)\exp(-x/L)$$

where x is the depth, $C_S$ and $C_B$ are the surface and bulk concentrations and L is the decay length in *Å*.

Note that the bulk concentration may be selected to be smaller or larger than the surface concentration and that the concentration profile in this way can be set to be either increasing or decreasing with the depth.

The structure can be changed by

Changing the **Surface Concentration**, the **Bulk concentration**, and **Decay Length**

To do this,

either

Click the respective text boxes and type the new values.

or

Click the Up-Down arrows next to the text boxes. The **Decay Length** changes each time the arrows are clicked by the amount in the textbox **Incr**. The increment may be changed by clicking the arrow next to the **Incr** textbox (see fig.4.9) and select a new value from the list. The Surface and Bulk concentration change by 0.05 for each click.

## 4.6 Several Buried Layers

This is used to analyze the peak shape and background from an in-depth concentration profile (see fig. 4.15) corresponding to several thin layers at different depths and with varying widths.

The algorithm used for this case assumes that the widths are small. It is a very good approximation when widths < 0.5 IMFP. The algorithms used for the other profiles in secs. 4.2-4.5 are exact (to within numerical limitations).

The user may investigate the accuracy of this approximation by analyzing a spectrum with the Buried Layer profile (which is based on an exact algorithm) with a delta function of the same width and the same depths.

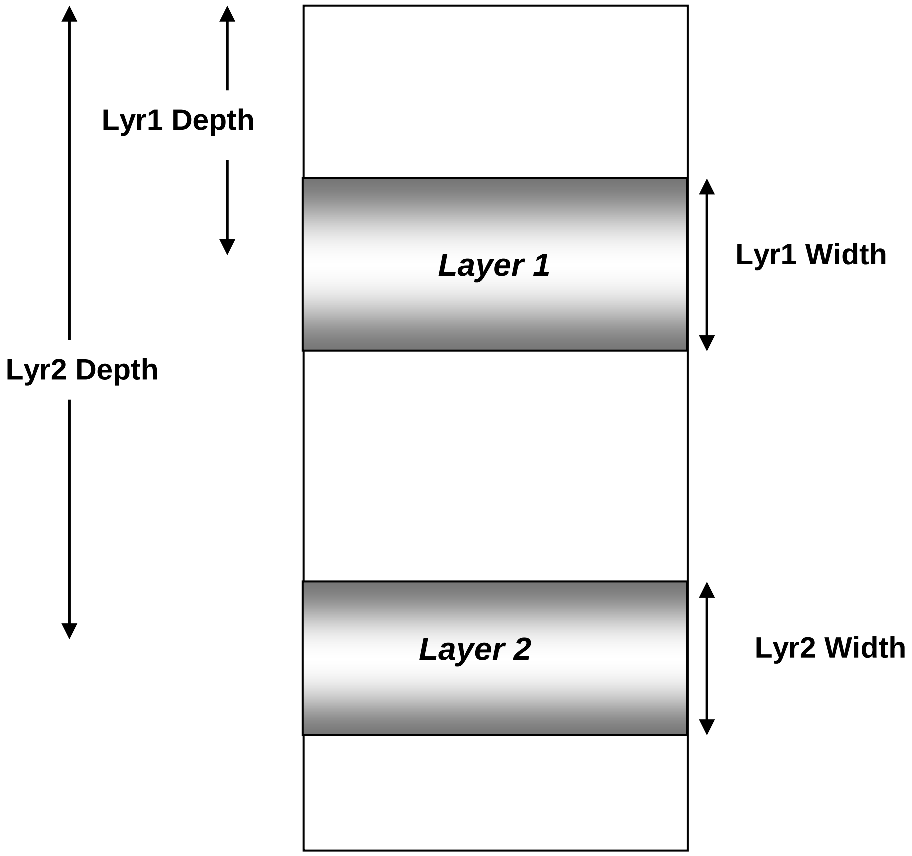


**Figure 4.15** In-depth concentration profile for **Several Buried Layers.**

Click the box labeled **Analyze**.

In the filelist, click the filename (e.g. Ag3d) with the XPS-spectrum.

Click **ReadSpec**.

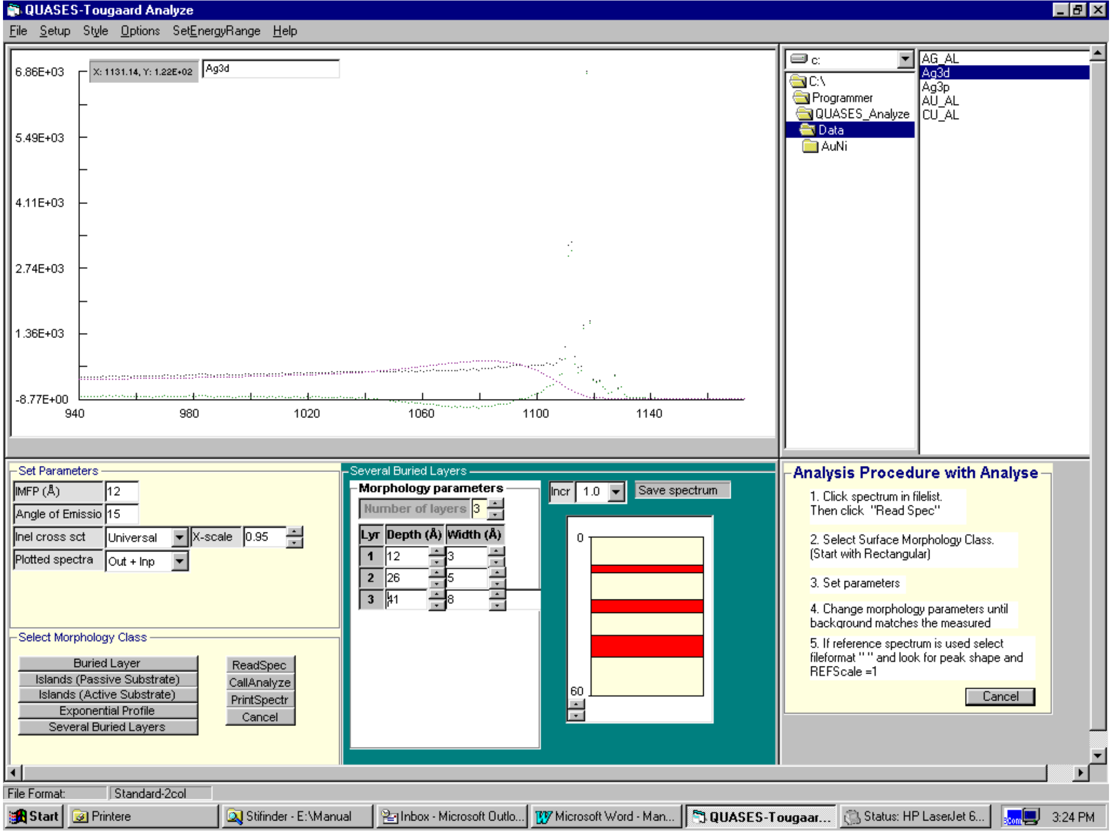
Click **Several Buried Layers** and get fig.4.16.

In the **Several Buried Layers – window** the

> **Number of layers** this number can be changed by clicking the Up-Down arrow.
>
> **Depth** is the depth in Å underneath the surface of the center of the layer.
>
> **Width** is the width in Å of this layer
>
> The **inset picture** gives a visualization of the surface structure.
>
> The maximum depth plotted in the inset picture may be changed by clicking the Up-Down arrow (see fig.4.2).

The structure can be changed by

> Changing the **Number of layers**. The maximum number of layers is 9.
>
> Changing the **Depth** of each layer
> Changing the **Width** of each layer
> The depth or width is changed by
>
> > either
> >
> > > Click the text box and type the depth and width
> >
> > or
> >
> > > Click the Up-Down arrows next to the text boxes. The depth/width changes each time the arrows are clicked by the amount in the textbox **Incr**. The increment may be changed by clicking the arrow next to the **Incr** textbox and select a new value from the list.
> >
> > (Note: the morphology can not be changed by dragging the mouse icon over the picture as in the case of a Buried Layer in Sec. 4.2)



IMFP (Å) 12

Angle of Emissio 15

Inel cross sct Universal

X-scale 0.95

Plotted spectra Out + Inp

Incr 1.0

Number of layers 3

| Lyr | Depth (Å) | Width (Å) |
|---|---|---|
| 1 | 12 | 3 |
| 2 | 26 | 5 |
| 3 | 41 | 8 |

**Analysis Procedure with Analyse**

1. Click spectrum in filelist.
Then click "Read Spec"

2. Select Surface Morphology Class.
(Start with Rectangular)

3. Set parameters

4. Change morphology parameters until
background matches the measured

5. If reference spectrum is used select
fileformat " " and look for peak shape and
REFScale =1

File Format: Standard-2col

Figure 4.16

# *Chapter 5*

# QUASES - Generate

The purpose of the program **QUASES-Generate** is to calculate model spectra for a given surface morphology. By comparing such model spectra to a measured spectrum from a solid with unknown composition, the in-depth concentration profile of atoms in the solid is determined.

The peak shape and background intensity of the model spectrum depends characteristically on the depth distribution of electron emitting atoms (see Chapter 1). This is illustrated in figs.1.1 and 1.2, which show the energy spectrum after passing different thickness. The user must therefore give information on the in-depth concentration profiles.

In the program **QUASES-Generate** this information is input in a quite similar way as in the program **QUASES-Analyze** (see Chapter 4). The depth concentration profiles have been divided into the same five main classes. Within each class, parameters to characterize the particular in-depth profile are specified.

The five classes of depth concentration profiles are

**Buried Layer**

**Islands (Passive Substrate)**

**Islands (Active Substrate)**

**Exponential Profile**

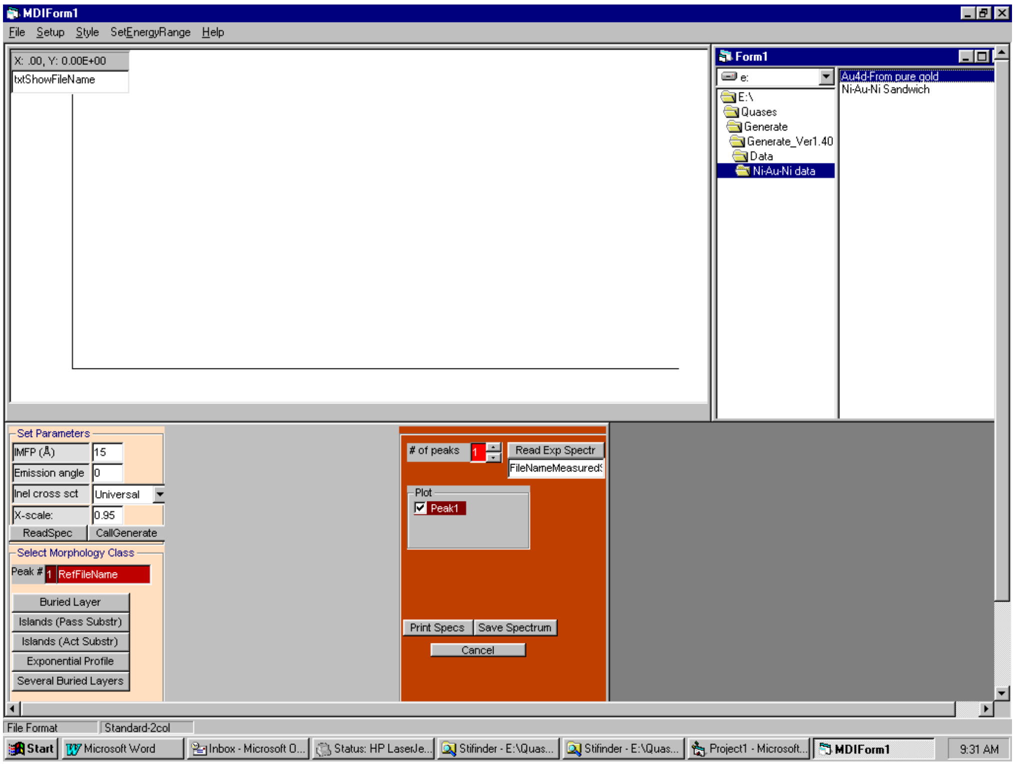
**Several Buried Layers**

Section 5.1 describes those parts of the menus in **QUASES-Generate** that are common to all depth profile classes and the parts that are specific to the individual classes are described in sections 5.2 - 5.6 below.

## 5.1 Menu items common to all QUASES-Generate depth profile classes

Start **QUASES-Generate** and get fig. 5.1.

The option **Correct** is described in Chapter 3 and the option **Tools** in Chapter 7.



X: .00, Y: 0.00E+00

txtShowFileName

IMFP (Å) 15

Emission angle 0

Inel cross sct Universal

X-scale: 0.95

Peak # 1

# of peaks 1

☑ Peak1

File Format Standard-2col

Click the box labeled **Generate** and get fig.5.2.

Here follows an explanation of those parameters that are common to all five depth profile classes.

### IMFP (Å)

This is the inelastic mean free path in Å for the moving electrons. To change the value, click the text box and type the new value.

### Angle of Emission

This is the angle, in degrees, of electron emission with respect to the surface normal. To change the value, click the text box and type the new value.

### Inelastic cross sct

This is used to specify the differential cross section for electron energy loss used to calculate the model spectrum. Click the arrow next to the text box to display a list of possible cross sections.

**Universal** (default value) is valid for transition metals and their oxides. This is a good choice in most cases.

**Polymer** should be used when analyzing spectra from polymers

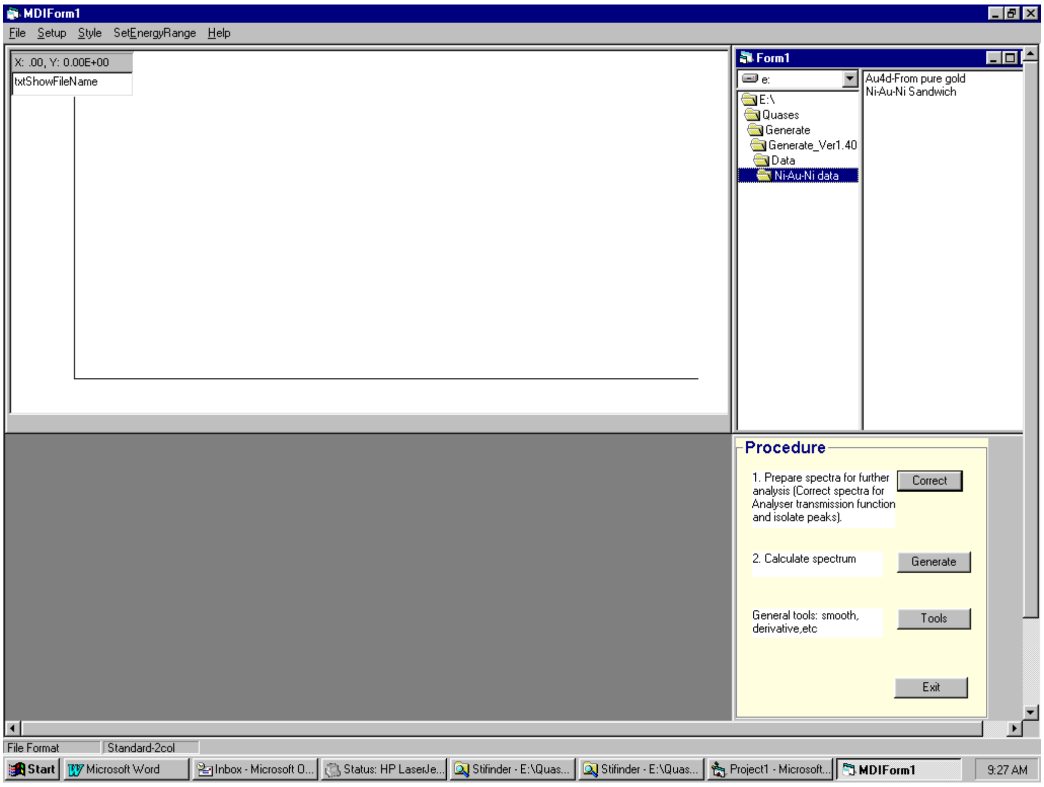
**SiO2** applies to $SiO_2$

**Si** applies to silicon

**Ge** applies to germanium

**Al** applies to aluminum

**File: x-sect**. Here the user can specify another cross section (e.g. determined from analysis of a REELS spectrum). This cross section should be saved under the filename x-sect in sub directory X-Sect. The required data format in the file with the cross section is described in Chapter 6.



1. Prepare spectra for further analysis (Correct spectra for Analyser transmission function and isolate peaks).

2. Calculate spectrum

General tools: smooth, derivative,etc

**Figure 5.1**

Select a cross section according to the nature of the solid under investigation by clicking the name of the cross section from the list.
Choose **Universal** if the solid does not fit into any of the listed possibilities.

### 2. X-scale

This is used to scale the cross section for inelastic electron scattering by the factor given in the textbox. Use a value around 0.95 unless other information on the value is available. The value may be changed by clicking the Up-Down arrows next to the textbox or by clicking within the textbox and type a new value.

## General remarks

The following steps are involved in the quantification with **QUASES-Generate** (see below for more details):

1. Read the spectrum from which the model spectrum will be calculated (see below)

2. Set parameters for the solid (*IMFP, Inel. Cross Sct*) and geometry (*Emission angle*)

3. Select one of the five classes of depth profiles.

4. Set the parameters that specify the surface structure.

This produces the model spectrum corresponding to the specified surface structure.

5. Read the measured spectrum from the sample with unknown surface composition.

6. Compare the shape and intensity of the model spectrum to the measured spectrum.

7. Change the surface morphology until there is an agreement between the model and the measured spectrum.

8. The true composition of the surface region of the unknown sample is equal to the thus determined structure.

**Note:**
The reference spectrum in Step 1 above must be of the following type:

For

**Buried Layer**

**Islands (Passive Substrate)**

**Islands (Active Substrate)**

**Exponential Profile**

the reference spectrum must be from a homogeneous solid.
This means the following: The model spectrum is calculated from a spectrum from a pure solid with a homogeneous in-depth distribution of atoms. Therefore for the **Buried Layer, Islands (Passive Substrate), Islands (Active Substrate), Exponential Profile** make sure that the spectrum which is read when clicking *ReadSpec* is the spectrum of the peak measured from a pure elemental solid.
This spectrum must first be corrected and the peak energy region isolated with the program *Correct* in the usual way (see Chapter 3).

3. When using **Several Buried Layers**, the reference spectrum must be from a background corrected spectrum.

This means the following: The spectrum from the depth profile class **Several Buried Layers** is calculated from an atomic F(E) spectrum. This is determined by the program **QUASES-Analyze** for example by analyzing a spectrum from a pure solid assuming a homogeneous in-depth concentration profile (e.g. by selecting the rectangular profile with **Start Depth**:0 and **End Depth**: 1000) or from analysis of any other spectrum from a solid with a well known in-depth profile.

> Therefore for the **Several Buried Layers** profile, make sure that the spectrum which is read when clicking **ReadSpec** has been background corrected by **QUASES-Analyze**.

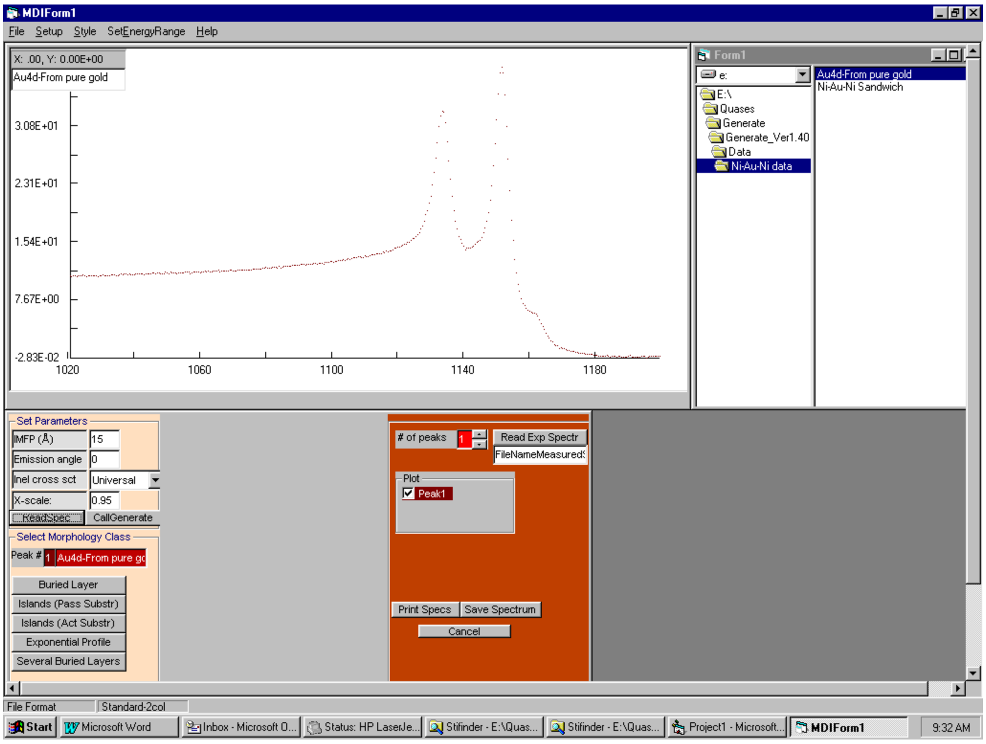
The point size used in the plot may be changed by selecting **Style** in the menu bar, select **Linewidth** and **Higher.**

Click the reference spectrum in the filelist (“Au4d From Pure Gold”)

Click **Read Spec** and get fig. 5.3

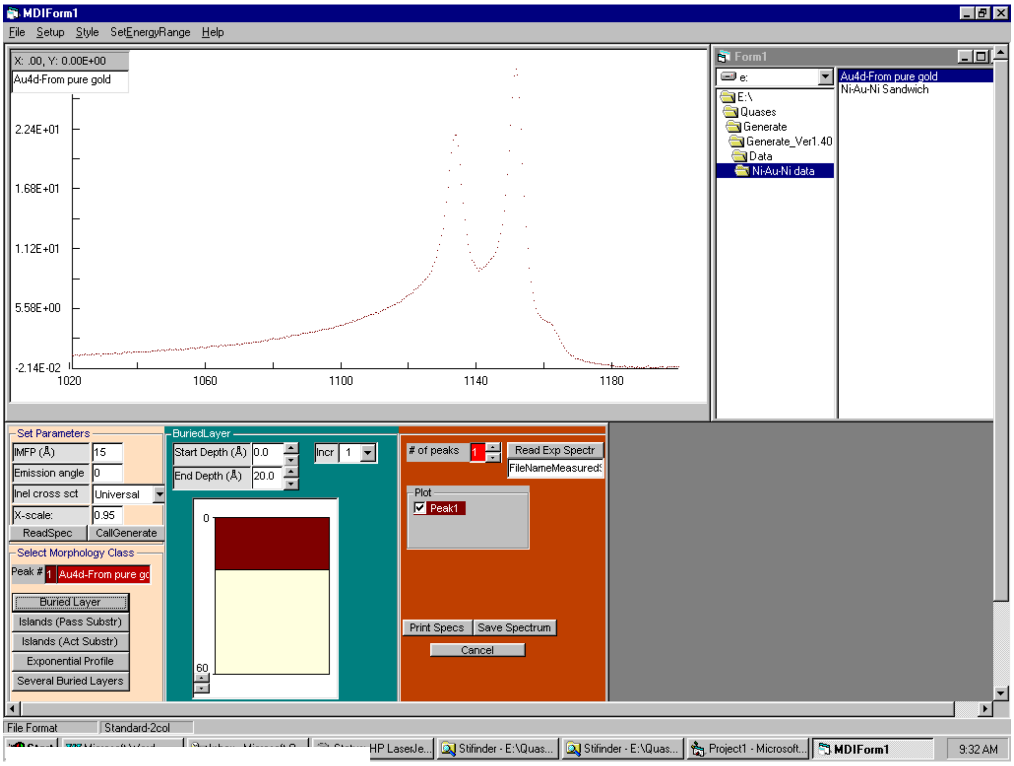
Click **Buried Layer** and get fig. 5.4.

The surface morphology may now be changed and the displayed spectrum is the model spectrum from a solid with this morphology.



IMFP (Å) 15
Emission angle 0
Inel cross sct Universal
X-scale: 0.95
Peak # 1 Au4d-From pure go
\# of peaks 1
☑ Peak1
File Format Standard-2col

## Figure 5.3



IMFP (Å) 15
Emission angle 0
Inel cross sct Universal
X-scale: 0.95
Peak # 1 Au4d-From pure gc
Start Depth (Å) 0.0
End Depth (Å) 20.0
Incr 1
\# of peaks 1
☑ Peak1
File Format Standard-2col

## Figure 5.4

## To compare the model spectrum to a spectrum from an unknown sample:

The generated model spectrum can be compared to a measured spectrum from an unknown solid. When a good fit to this spectrum has been found, the surface morphology of the unknown solid has been quantified.

**Note:** The measured spectrum must first be corrected and the peak energy region isolated with the program **Correct** in the usual way (see Chapter 3).

Do the following to read the experimental spectrum:

1. In the filelist, click the filename with the spectrum then click **Read Exp Spectr**. The spectrum is then displayed and the filename appears in the textbox below the **Read Exp Spectr** button.

2. If there is an energy shift between the model spectrum and the experimental spectrum, this can be corrected for by changing the value of **Eshift** (see fig.5.5). **Eshift** may be changed either by clicking within the textbox and typing the new value or by using the Up-Down arrows next to the **Eshift** textbox. Each mouse click changes **Eshift** by ± 0.5 eV.

In the plot with the experimental and model spectra there now appears two vertical lines. The position of these lines may be changed with the mouse by positioning the mouse icon over one of the lines, then click and hold the left mouse button and drag the line to the new position.

Three new textboxes also appear in the **Center window**:

**E1** is the energy position of the left line

**E2** is the energy position of the right line

**Ap** is the peak area of the generated model spectrum in the energy region from **E1** to **E2**.

**Scale** is the peak area ratio of the model spectrum to the experimental spectrum within the energy range from **E1** to **E2**.

$$Scale = \frac{\sum x(i) \cdot \Delta E}{\sum z(i) \cdot \Delta E_{ref}}$$

where x(i) is the experimental spectrum and z(i) the model spectrum and $\Delta E$ and $\Delta E_{ref}$ are the respective energy steps.

The experimental spectrum is divided by **Scale** before it is plotted.

## To calculate a model spectrum from more than one type of atom:

If the experimental spectrum has peaks that originate from different atoms, this can be modelled by clicking the UpDown arrow next to **# of peaks** . This opens a new window (see fig.5.6) where the peak and the morphology for the other type of atoms can be specified. Click once more and  a third window appears. It is thus possible to model a spectrum, which has peaks that originate from up to three different types of atoms.

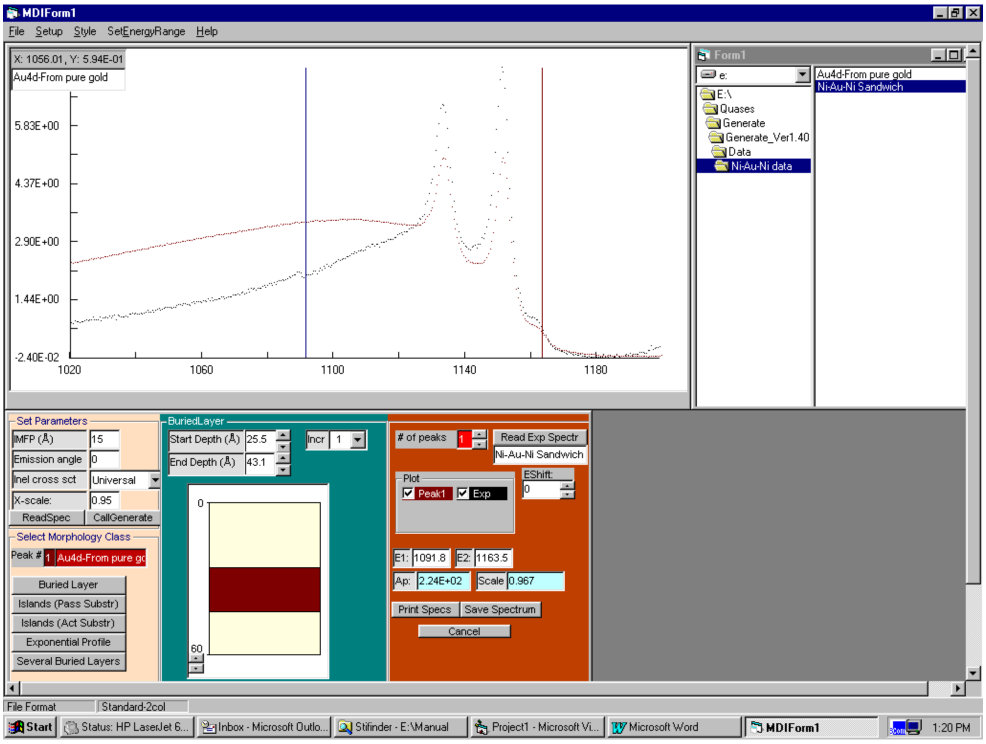
### Print the spectra.

To print the spectra displayed on the plot screen, click the **PrintSpectr** button.

### Save spectrum

To save the background corrected spectrum click **Save Spectrum.**
Type any comments that you may wish to store with the spectrum and type a filename.
Click **Save spectrum**. The new filename appears in the filelist box.

The following sections describe details of the procedures used to generate model spectra for the five classes of depth profiles.



X: 1056.01, Y: 5.94E-01

Au4d-From pure gold

IMFP (Å) 15

Emission angle 0

Inel cross sct Universal

X-scale: 0.95

Peak # 1 Au4d-From pure go

Start Depth (Å) 25.5

End Depth (Å) 43.1

Incr 1

# of peaks 1

Ni-Au-Ni Sandwich

EShift: 0

E1: 1091.8 E2: 1163.5

Ap: 2.24E+02 Scale 0.967

File Format Standard-2col

Figure 5.5

## 5.2 Buried Layer.

This is used to generate model spectra from rectangular in-depth concentration profiles. The upper and lower bounds of the rectangular profile can be chosen arbitrarily and it can therefore be used to model a large variety of profiles including substrates with an overlayer, an overlayer on a substrate, a buried layer, and a homogeneous solid. This profile is therefore a good starting point when the a spectrum from an unknown solid is modeled.

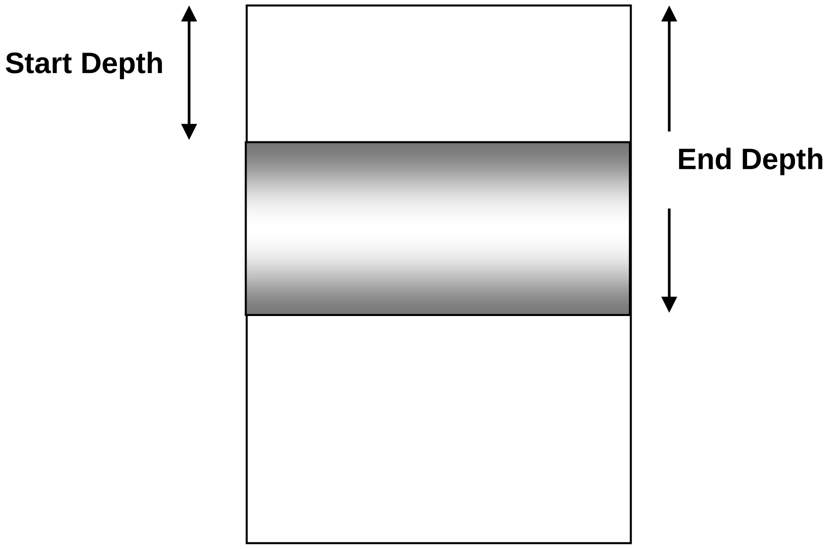


**Figure 5.6**

Click the box **Generate**.

In the filelist, click the filename (here ”Au4d From pure Gold”) with a spectrum from pure gold in the Au4d energy range (for details see page 59).

Click **ReadSpec** and get fig.5.3.

Click **Buried Layer** and get fig.5.4.

In the **Buried Layer – window** the

**Start Depth** is the depth in Å where the buried layer starts

**End Depth** is the depth in Å where the buried layer ends.

The **inset picture** gives a visualization of the surface structure.

The maximum depth plotted in the inset picture may be changed by clicking the Up-Down arrow (see fig.4.2).

There are three ways to change the in-depth concentration profile.

Either

- Click the text box and type the new **Start Depth** or **End Depth**.

or

- Click the Up-Down arrows next to the text boxes. The increments each time the arrows are clicked is given by the increment in the textbox *Incr*. The increment may be changed by clicking the arrow next to the *Incr* textbox (see fig.4.9) and select a new value from the list.

or

- Move the mouse over the region of the Start or End depth in the inset picture. The mouse icon changes to an arrow (see fig.4.2). Now click the left mouse button, hold the button and drag the mouse icon to the new desired depth and finally release the mouse button.

or

- Move the mouse over the center depth of the rectangular profile. The mouse icon changes to an arrow. Now click the left mouse button, hold the button and drag the mouse icon to the new desired depth and finally release the mouse button.

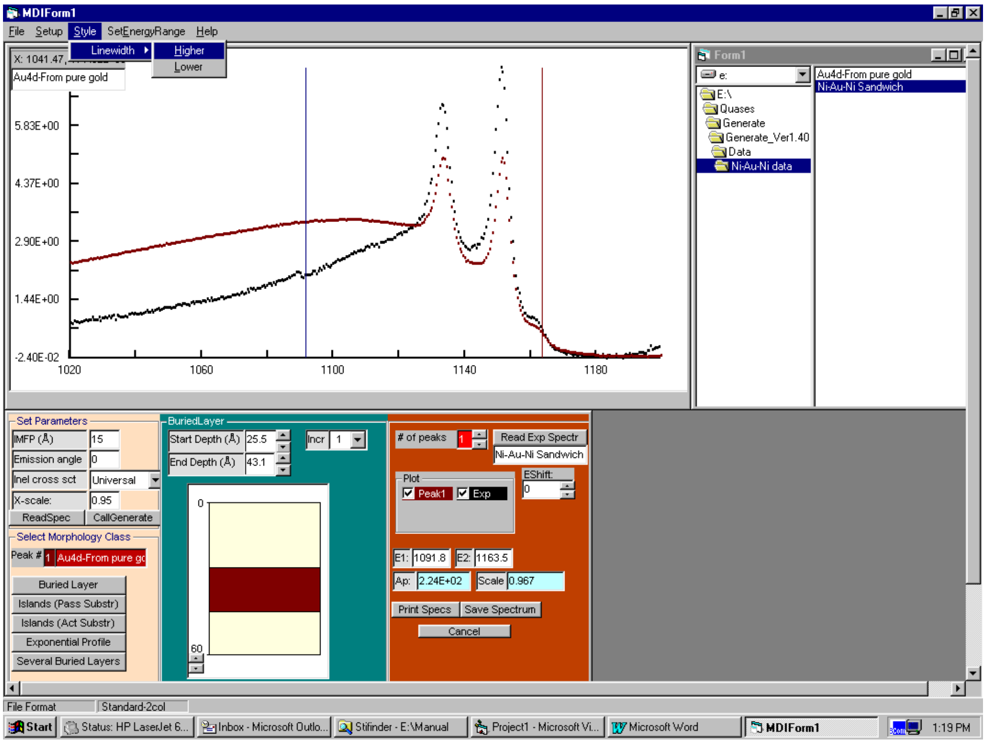
The model spectrum is calculated from the morphology specified in the **Buried Layer** window and the parameters that are set in the **Set Parameter window**.

Whenever a parameter is changed, the calculation is updated and the new model spectrum is plotted.

## Comparing the model spectrum to a measured spectrum

To determine the in-depth concentration profile of atoms in an unknown solid the generated model spectrum is compared to the measured spectrum from that solid. Do the following to do this comparison:

- In the filelist, click the file with the spectrum (here: “Ni-Au-Ni Sandwich”).



X: 1041.47,

Au4d-From pure gold

e:

E:\

Au4d-From pure gold
Ni-Au-Ni Sandwich

IMFP (Å) 15
Emission angle 0
Inel cross sct Universal
X-scale: 0.95

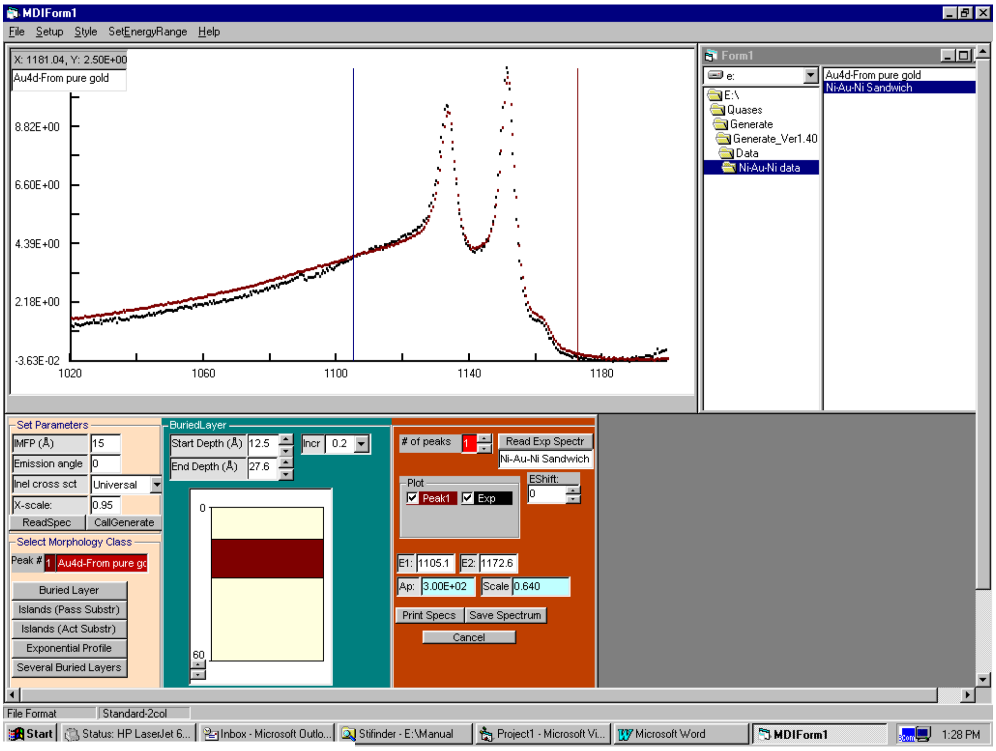
Peak # 1 Au4d-From pure go

Start Depth (Å) 25.5
End Depth (Å) 43.1
Incr 1

# of peaks 1
Ni-Au-Ni Sandwich
☑ Peak1 ☑ Exp
EShift: 0
E1: 1091.8 E2: 1163.5
Ap: 2.24E+02 Scale 0.967

File Format Standard-2col

Figure 5.7



X: 1181.04, Y: 2.50E+00

Au4d-From pure gold

e:

E:\

Au4d-From pure gold
Ni-Au-Ni Sandwich

IMFP (Å) 15
Emission angle 0
Inel cross sct Universal
X-scale: 0.95

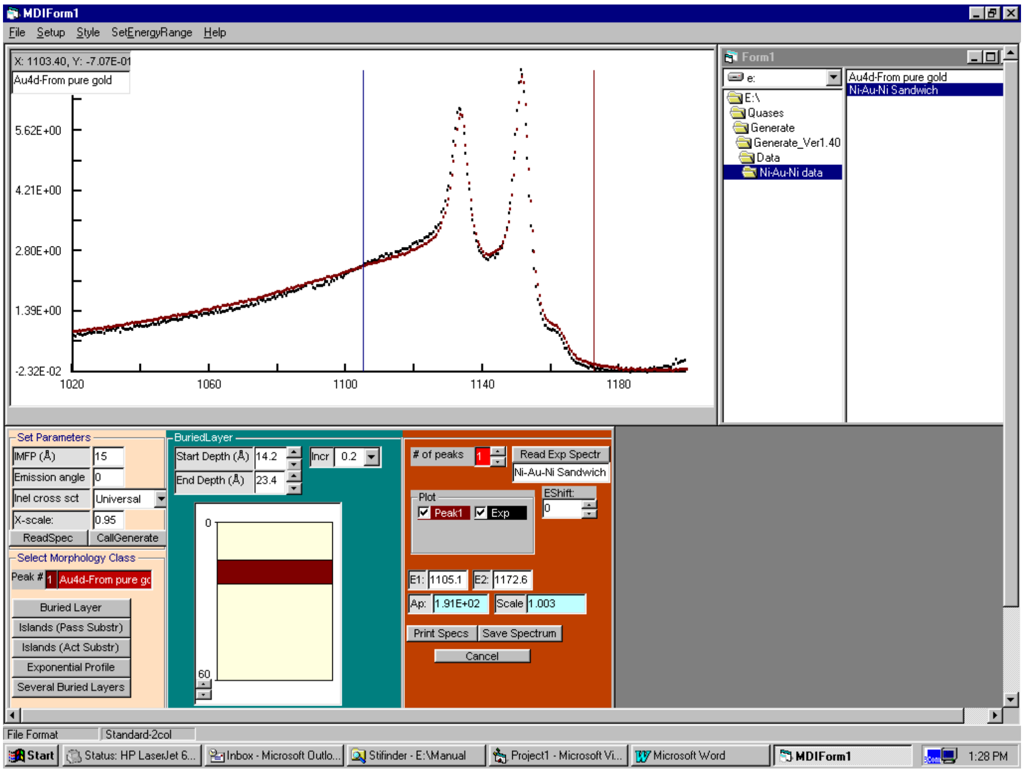
Peak # 1 Au4d-From pure go

Start Depth (Å) 12.5
End Depth (Å) 27.6
Incr 0.2

# of peaks 1
Ni-Au-Ni Sandwich
☑ Peak1 ☑ Exp
EShift: 0
E1: 1105.1 E2: 1172.6
Ap: 3.00E+02 Scale 0.640

File Format Standard-2col

Figure 5.8



X: 1103.40, Y: -7.07E-01

Au4d-From pure gold

Set Parameters

IMFP (Å) 15

Emission angle 0

Inel cross sct Universal

X-scale: 0.95

Peak # 1 Au4d-From pure go

Start Depth (Å) 14.2

End Depth (Å) 23.4

Incr 0.2

\# of peaks 1

Ni-Au-Ni Sandwich

☑ Peak1 ☑ Exp

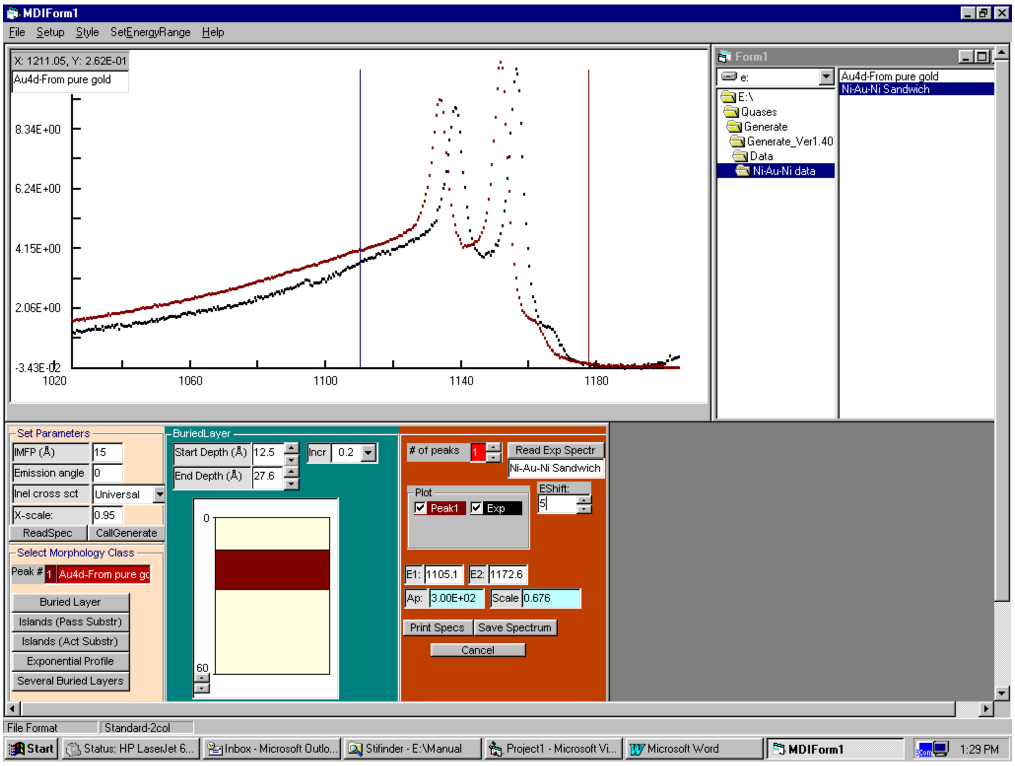
EShift: 0

E1: 1105.1 E2: 1172.6

Ap: 1.91E+02 Scale 1.003

File Format Standard-2col

## Figure 5.9



X: 1211.05, Y: 2.62E-01

Au4d-From pure gold

Set Parameters

IMFP (Å) 15

Emission angle 0

Inel cross sct Universal

X-scale: 0.95

Peak # 1 Au4d-From pure go

Start Depth (Å) 12.5

End Depth (Å) 27.6

Incr 0.2

\# of peaks 1

Ni-Au-Ni Sandwich

☑ Peak1 ☑ Exp

EShift: 5

E1: 1105.1 E2: 1172.6

Ap: 3.00E+02 Scale 0.676

File Format Standard-2col

## Figure 5.10

- Click **Read Exp Spectr**. and get fig.5.5.

- Change the **Start Depth** and **End Depth** until a good fit is obtained (see figs.5.7 and 5.8).

- With the mouse, move the two vertical lines in the plot so they cover the main part of the peak structure. Note that **Scale** differs from 1.00. This is because the thickness of the in depth profile in fig.5.7 is still off (by the factor **Scale**).

- Change the **Start Depth** and **End Depth** until **Scale** is ~ 1.00 (see fig.5.9)

The surface morphology of the sample from which the spectrum was measured is equal to the determined structure.

The gold atoms in the sample has thus been determined to form a layer that extends from 14.2 Å to 23.4 Å underneath the surface.

Explore the effect of **Eshift** by clicking the UpDown arrows (see fig.5.10).

## 5.3 Islands (Passive Substrate)

This is used to generate model spectra from a depth profile of islands (see fig. 5.11). **Island (Passive Substrate)** calculates the spectrum of electrons emitted from the overlayer atoms. Another option **Islands (Active Substrate)** calculates the spectrum of electrons emitted from the substrate atoms of a similar structure (see Section 5.4 below).

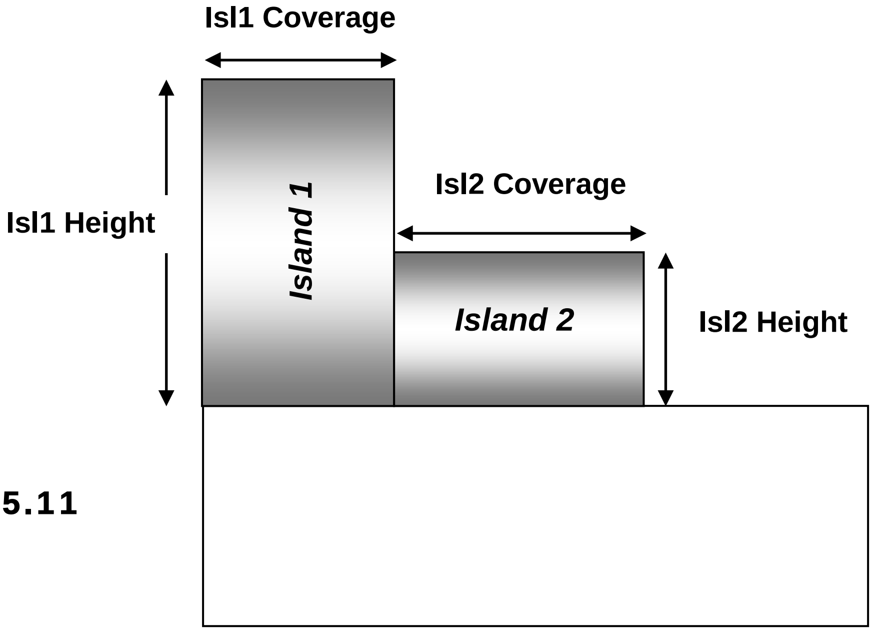


**Figure 5.11**

Click **Generate**
In the filelist, click the filename (here ”Au4d From pure Gold”) with a spectrum from pure gold in the Au4d energy range (for details see page 59).

Click **ReadSpec**

Click **Islands (Passive Substrate)** and get fig.5.12.

In the **Islands (Passive Substrate) – window** the following parameters can be set.

> **Number of islands.** This number can be changed by clicking the Up-Down arrow.
>
> **Height** is the height in Å of each island
>
> **Coverage** is the fraction of the surface covered by the island
>
> The **inset picture** gives a visualization of the surface structure.
>
> The maximum depth plotted in the inset picture may be changed by clicking the Up-Down arrow.

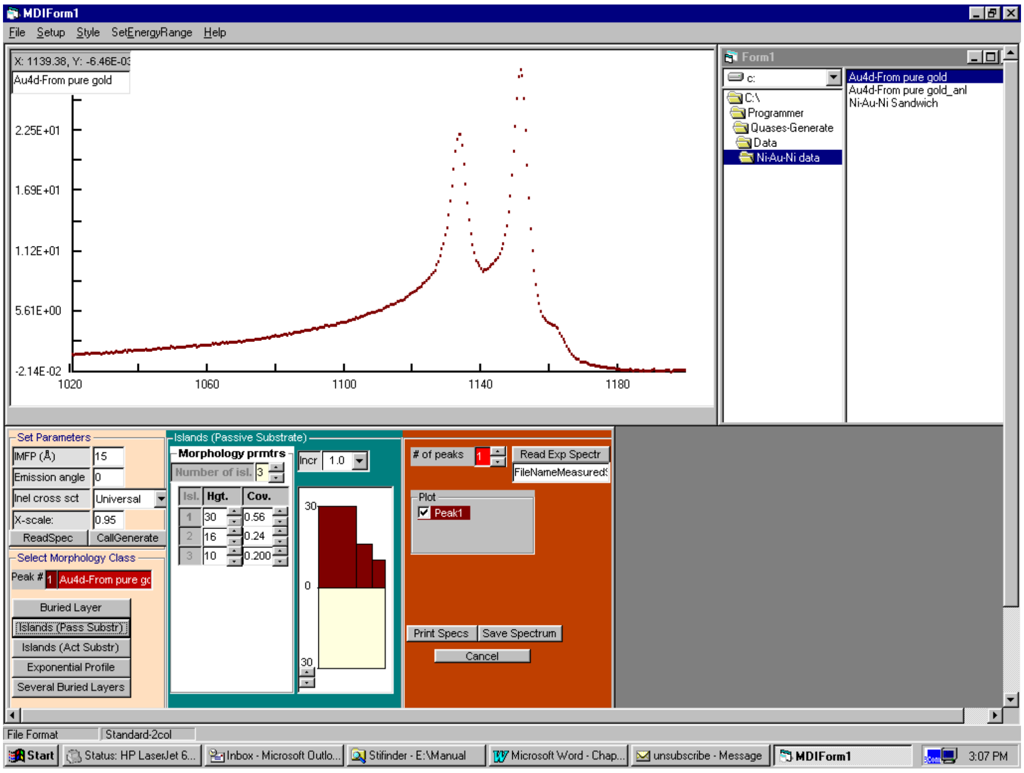
If the selected total coverage exceeds 1, the program recalculates the coverage of the last island to fulfill the constraint that the total coverage cannot exceed 1.

To model a structure with islands that cover a total of less than 1, set the height of the last island to zero.

The island structure can be changed by

> Changing the **Number of islands**. The maximum number of islands is 9.
>
> Changing the **Height** and **Coverage** of each island
> To do this,
>
> either
>
> Click the text box and type the new **Height** and **Coverage**.
> or
>
> Click the Up-Down arrows next to the text boxes. The height changes each time the arrows are clicked by the increment in the textbox **Incr**. The increment may be changed by clicking the arrow next to the **Incr** textbox (see fig.4.9) and select a new value from the list. The coverage changes by 0.05 for each mouse click.

(**Note:** the morphology can not be changed by dragging the mouse icon over the picture as in the case of a Buried Layer in Sec. 5.2)



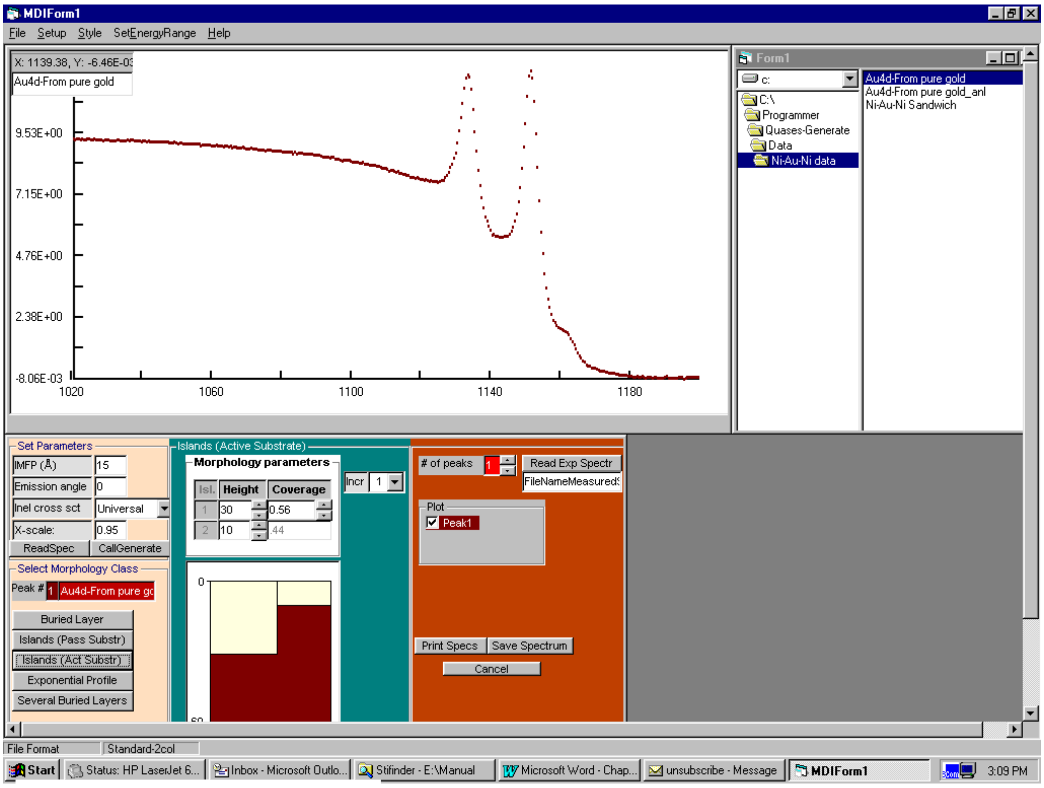
X: 1139.38, Y: -6.46E-03

Au4d-From pure gold

IMFP (Å) 15
Emission angle 0
Inel cross sct Universal
X-scale: 0.95
Peak # 1 Au4d-From pure go
Number of isl. 3
Incr 1.0
# of peaks 1
FileNameMeasured
File Format Standard-2col

| Isl. | Hgt. | Cov. |
|---|---|---|
| 1 | 30 | 0.56 |
| 2 | 16 | 0.24 |
| 3 | 10 | 0.200 |

Figure 5.12



X: 1139.38, Y: -6.46E-03

Au4d-From pure gold

IMFP (Å) 15
Emission angle 0
Inel cross sct Universal
X-scale: 0.95
Peak # 1 Au4d-From pure go
Incr 1
# of peaks 1
FileNameMeasured
File Format Standard-2col

| Isl. | Height | Coverage |
|---|---|---|
| 1 | 30 | 0.56 |
| 2 | 10 | 44 |

Figure 5.14

## 5.4 Islands (Active Substrate)

This is used to generate model spectra from a substrate that is covered by an overlayer of islands. **Island (Active Substrate)** is used to calculate the spectrum from the substrate atoms after they have passed through the overlayer islands (see fig. 5.13). Another depth profile class **Island (Passive Substrate)** is used to calculate the spectrum from the overlayer atoms of a similar island structure (see Section 5.3).

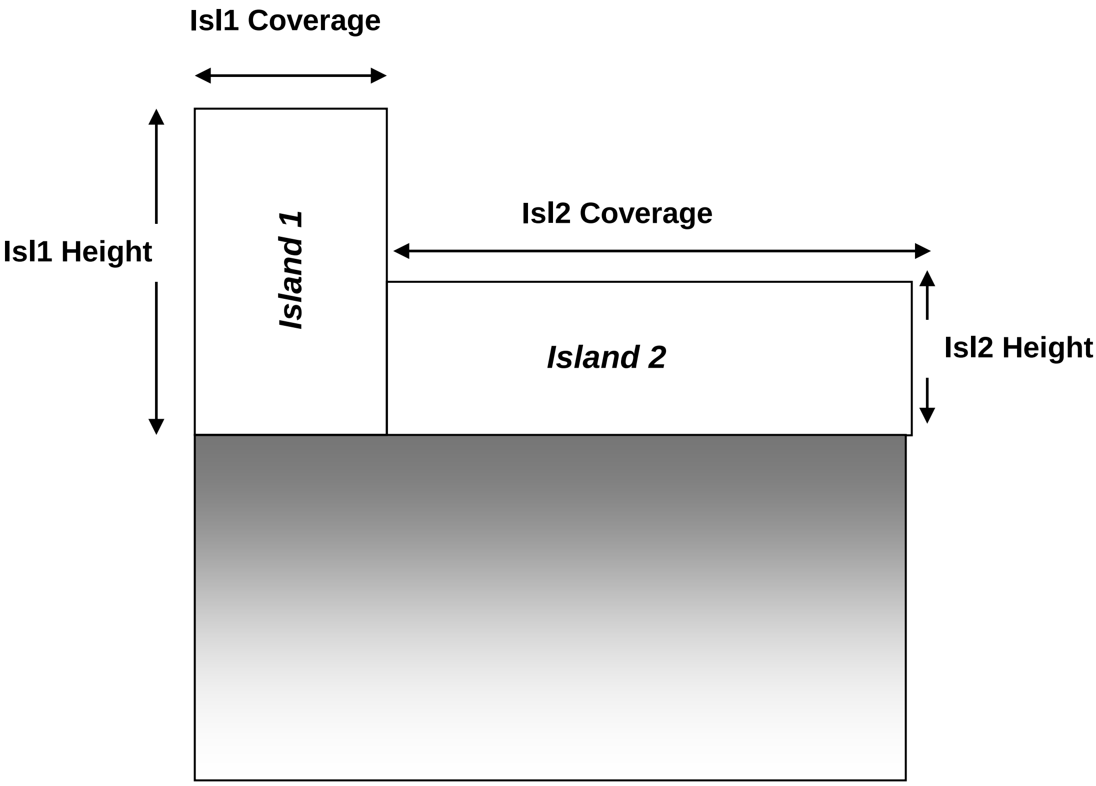


**Figure 5.13** The height and coverage of the two islands.

Click **Generate**.
In the filelist, click the filename (here ”Au4d From pure Gold”) with a spectrum from pure gold in the Au4d energy range (for details see page 59).

Click **ReadSpec**

Click **Islands (Active Substrate)** and get fig.5.14.

In the **Islands (Active Substrate) – window** the

> **Height** is the height in Å of each of the two islands.
>
> **Coverage** is the fraction of the surface covered by this island
>
> The **inset picture** gives a visualization of the surface structure.
>
> By clicking the Up-Down arrow (see fig.4.2), the maximum depth plotted in the inset picture may be changed.

To model the effect of a single island, set the height of island 2 to zero.

**Note that the number of islands is limited to two. This can not be changed.**

The structure can be changed by

> Changing the **Height** and **Coverage** of each island
> To do this,
>
> either
>
> Click the text box and type the new **Height** and **Coverage**.
>
> or
>
> Click the Up-Down arrow next to the text boxes. The height changes each time the arrows are clicked by the amount in the textbox **Incr**. The increment may be changed by clicking the arrow next to the **Incr** textbox (see fig.4.9) and select a new value from the list. The coverage changes by 0.05 for each mouse click.
>
> (**Note**: the morphology can not be changed by dragging the mouse icon over the picture as in the case of a Buried Layer in Sec. 5.2)

## 5.5 Exponential Profile.

This is used to generate model spectra from exponential in-depth concentration profiles (see fig.5.15). The profile may be either exponentially increasing or decreasing with depth and the surface and the bulk concentrations may have any value between 0 and 1.

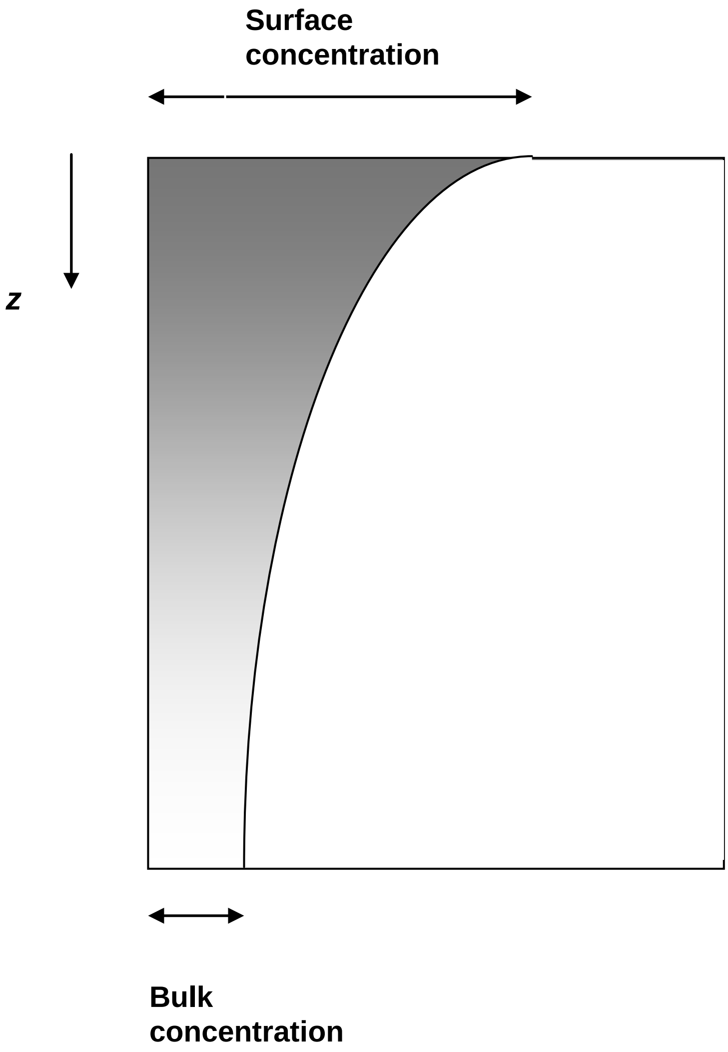


**Figure 5.15** Exponential depth profiles.

Click **Generate**.

In the filelist, click the filename (here ”Au4d From pure Gold”) with a spectrum from pure gold in the Au4d energy range (for details see page 59).

Click **ReadSpec**

Click **Exponential Profile** and get fig.5.16.

In the **Exponential Profile – window** the

> **Surface concentration** is the concentration at the surface (value between 0 and 1. If the input is outside of this range, the program selects the nearest allowed value).
>
> **Bulk concentration** is the concentration deep in the bulk (value between 0 and 1. If the input is outside of this range, the program selects the nearest allowed value).
>
> **Decay length** is the decay length in Å of the exponential profile.
>
> The **inset picture** gives a visualization of the surface structure.
>
> The maximum depth plotted in the inset picture may be changed by clicking the Up-Down arrow (see fig.4.2).

The concentration profile is

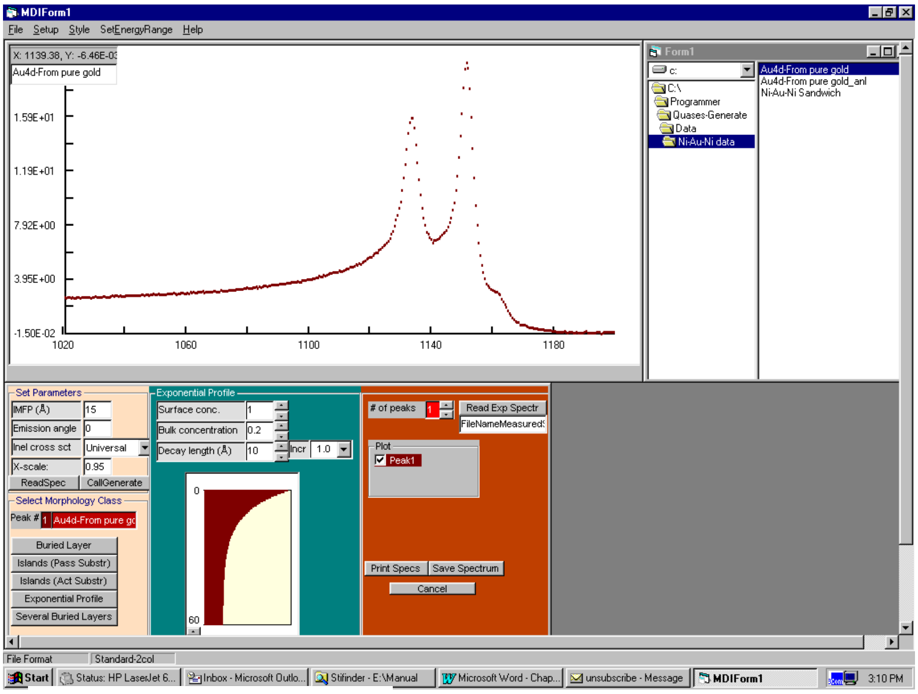
$$f(z) = C_B + (C_S - C_B)\exp(-z/L)$$

where *z* is the depth, $C_S$ and $C_B$ are the surface and bulk concentrations and L is the decay length in *Å*.

Note that the bulk concentration may be selected to be smaller or larger than the surface concentration and that the concentration profile in this way can be set to be either increasing or decreasing with the depth.

The structure can be changed by

> Changing the **Surface Concentration**, the **Bulk concentration**, and **Decay Length**
>
> To do this,
>
> either



X: 1139.38, Y: -6.46E-03

Au4d-From pure gold

IMFP (Å) 15

Emission angle 0

Inel cross sct Universal

X-scale: 0.95

Surface conc. 1

Bulk concentration 0.2

Decay length (Å) 10

Incr 1.0

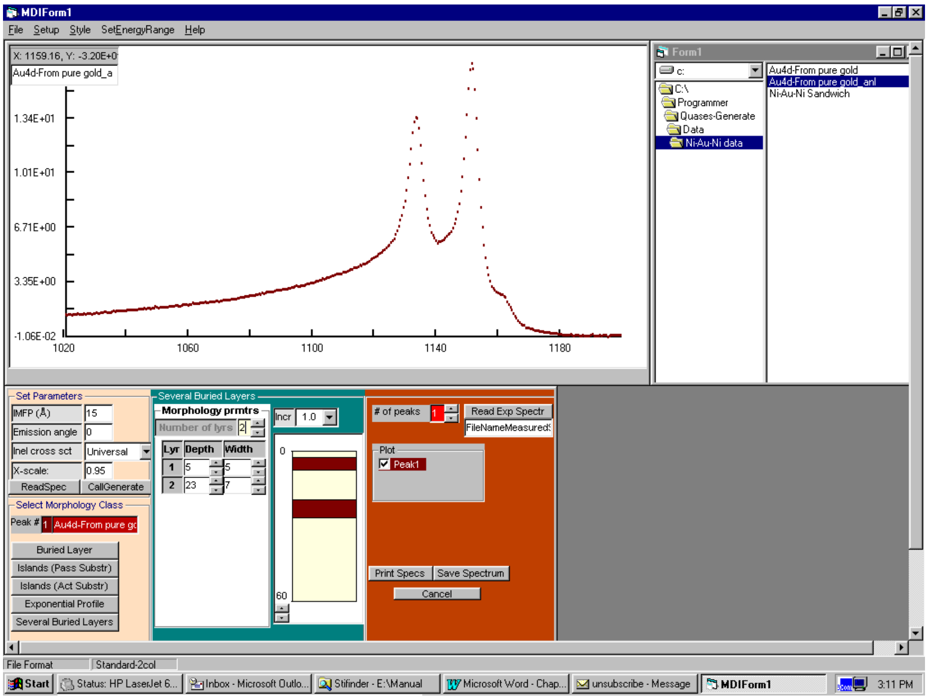
# of peaks 1

Peak # 1 Au4d-From pure gold

☑ Peak1

File Format Standard-2col

Figure 5.16



X: 1159.16, Y: -3.20E+0

Au4d-From pure gold_a

IMFP (Å) 15

Emission angle 0

Inel cross sct Universal

X-scale: 0.95

Number of lyrs 2

Incr 1.0

| Lyr | Depth | Width |
|---|---|---|
| 1 | 5 | 5 |
| 2 | 23 | 7 |

# of peaks 1

Peak # 1 Au4d-From pure gc

☑ Peak1

File Format Standard-2col

Figure 5.17

Click the respective text boxes and type the new values.

or

Click the Up-Down arrows next to the text boxes. The **Decay Length** changes each time the arrows are clicked by the amount in the textbox **Incr**. The Increment may be changed by clicking the arrow next to the **Incr** textbox (see fig.4.9) and select a new value from the list. The **Surface** and **Bulk concentration** change by 0.05 for each click.

## 5.6 Several Buried Layers

This is used to generate model spectra from in-depth concentration profiles (see fig. 5.18) that consist of several thin layers at different depths and with varying widths.

The algorithm used for this case assumes that the widths are small. It is a very good approximation when widths < 0.5 IMFP. The algorithms used for the other profiles in Secs. 5.2-5.5 are exact (to within numerical limitations).

The accuracy of this approximation can be investigated by generating a spectrum from the Buried Layer profile in Sec.5.2 (which is based on an exact algorithm) with the spectrum mede with **Several Buried Layers** using one layer of the same width and the same depths.

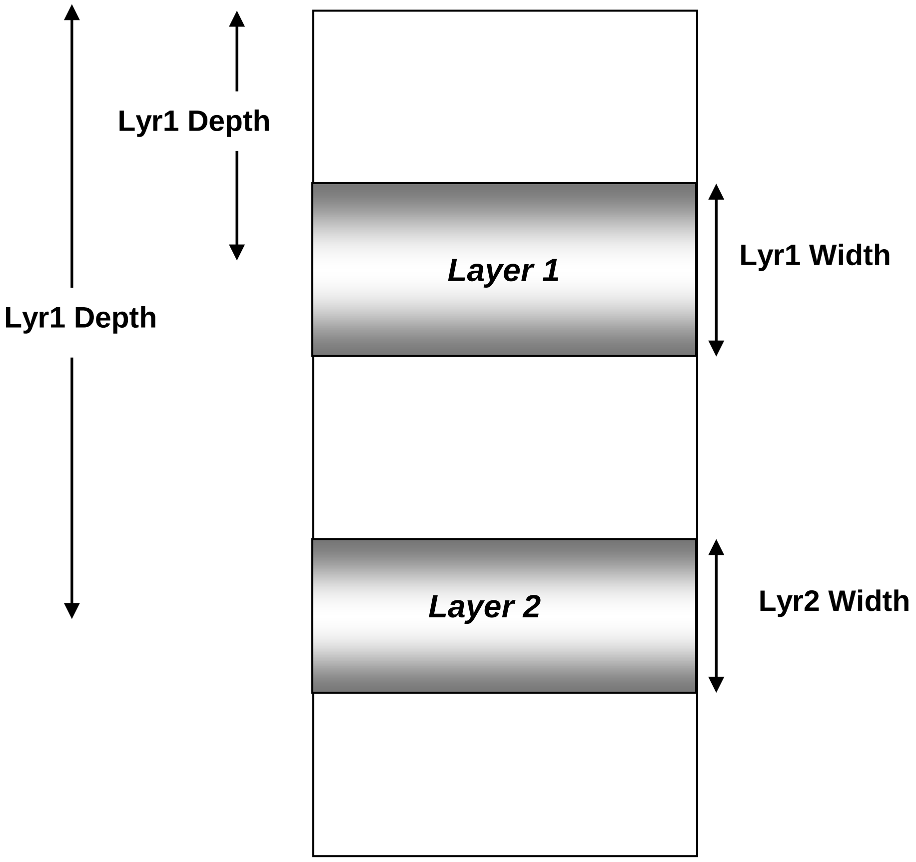


**Figure 5.18**

Click **Generate**.
In the filelist, click the filename (here ”Au4d From pure Gold_anl”) with a spectrum from pure gold in the Au4d energy range that has been background corrected by QUASES-analyze (for details see page 59). See below for information on how this is determined.

Click **ReadSpec**

Click **Several Buried Layers** and get fig.5.17.

In the **Several Buried Layers – window** the following parameters can be set:

**Number of layers.** This number can be changed by clicking the Up-Down arrow.

**Depth** is the depth in Å underneath the surface of the center of the layer.

**Width** is the width in Å of the layer

The **inset picture** gives a visualization of the surface structure.

The maximum depth plotted in the inset picture may be changed by clicking the Up-Down arrow.

The structure can be changed by

Changing the **Number of layers**. The maximum number of layers is 9.

Changing the **Depth** of each layer

Changing the **Width** of each layer

The **Depth** or **Width** is changed by

either

Click the text box and type the depth and width

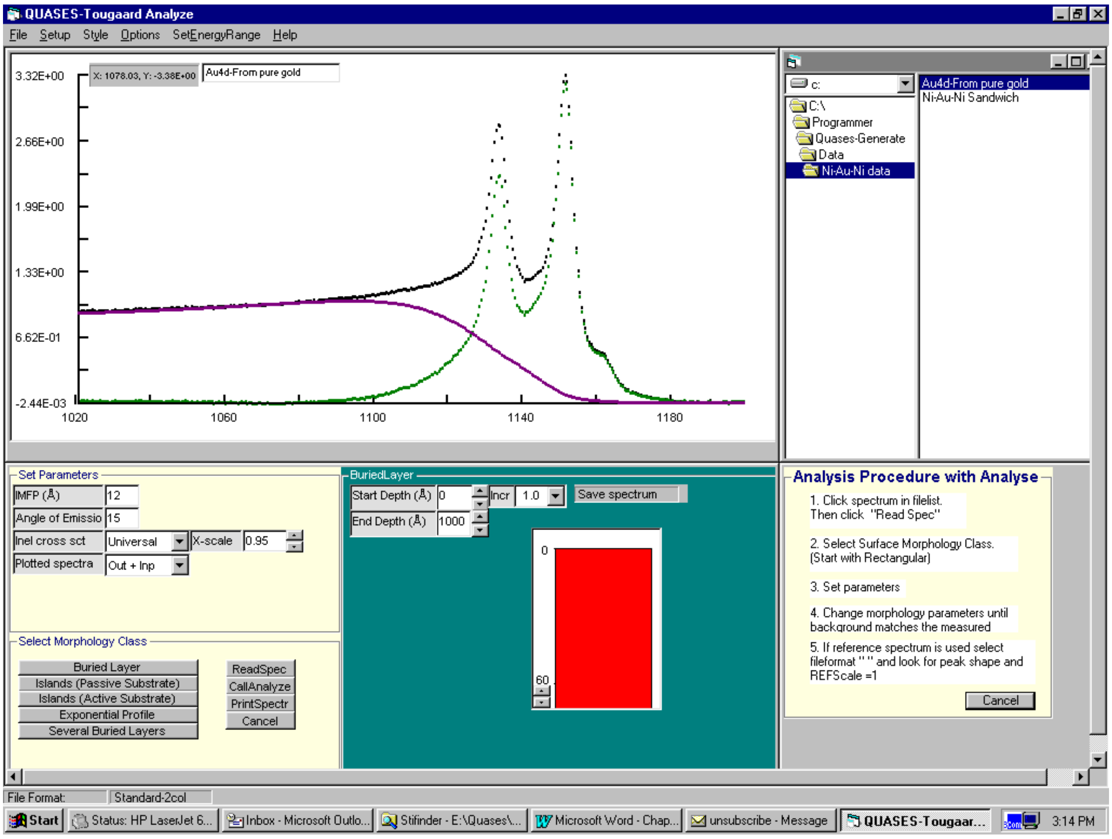
or

Click the Up-Down arrows next to the text boxes. The depth/width changes each time the arrows are clicked by the amount in the textbox **Incr**. The Increment may be changed by clicking the arrow next to the **Incr** textbox and select a new value from the list.

(**Note**: the morphology can not be changed by dragging the mouse icon over the picture as in the case of a Buried Layer in Sec. 5.2)

# Determination of the input spectrum used in Several Buried Layers.

1. Start **QUASES-Analyze**
2. Click **Analyze**.
3. Click the file ”Au4d From pure Gold” in the filelist.
4. Click **Buried Layer**. See fig. 5.19
5. Set **Start Depth** = 0 and **End Depth** = 1000.
6. If necessary, change **Scale** so the background meets the measured spectrum below the peak.
7. Click **Save Spectrum** and save the spectrum.
8. The filename: ”Au4d From pure Gold_anl” appears in the filelist.



IMFP (Å) 12
Angle of Emissio 15
Inel cross sct Universal
X-scale 0.95
Plotted spectra Out + Inp
Start Depth (Å) 0
Incr 1.0
End Depth (Å) 1000
File Format: Standard-2col

**Analysis Procedure with Analyse**

1. Click spectrum in filelist. Then click "Read Spec"
2. Select Surface Morphology Class. (Start with Rectangular)
3. Set parameters
4. Change morphology parameters until background matches the measured
5. If reference spectrum is used select fileformat " " and look for peak shape and REFScale =1

**Figure 5.19**

# Chapter 6

# File Formats and File Management

**Note:** The programs assume that the American standard for numbers is used (where the decimal place is marked by a ".") and will not run properly if setting is different. To change settings, select Start on the Windows menu bar and then select Settings, Control Panel, Regional Settings, English (United States) . Alternatively, you may change the number settings for your current Regional settings to the American standard.

It is helpful to be able to keep track of the experimental data files as well as of the files created by the programs. For example, by application of the program **Correct** you will create new datafiles which are used as input files in the program **QUASES-Analyze** or **QUASES-Generate**.

The data format of the files is described below. If problems are met in the execution of the programs it may be necessary to check the data format and maybe to make changes to the files to make them consistent with the selected data format.

To facilitate these operations, a file managment system has been developed for QUASES.

On  right hand side of the **Main Menu** is the **File Manager** (see fig. 6.1). It consists of three boxes which list the **DiskDrive**, the **Directories** and the **FileNames.**

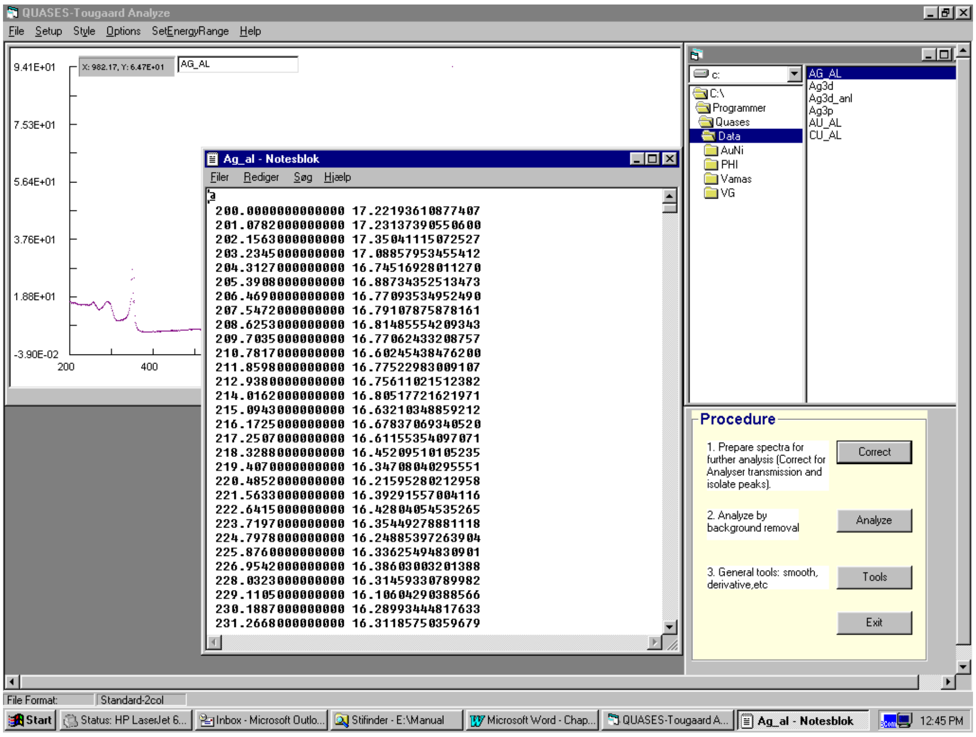
The **DiskDrive** displays the current drive. Clicking the arrow on the right of the DiskDrive box, the box drops down and displays all valid drives on your system. You can select a new drive from the list which will then appear in the **DiskDrive** box.

The **Directory** box displays the directory structure of the current drive. You may move up and down in the list of directories or use the scroll bar at the right of the box. By double-clicking a directory the box will display the selected directory and its subdirectories. The Filelist list box to the far right shows the files in the current directory.

## Edit

*The easiest way to **Edit** a file is by simply double-clicking the filename in the **FileList** box.*

This opens the file with the Notebook editor which provides all the well known facilities for file editing, saving, printing etc. To exit the editor, select Exit from the File menu.



```
a
 200.0000000000000 17.22193610877407
 201.0782000000000 17.23137390550600
 202.1563000000000 17.35041115072527
 203.2345000000000 17.08857953455412
 204.3127000000000 16.74516928011270
 205.3908000000000 16.88734352513473
 206.4690000000000 16.77093534952490
 207.5472000000000 16.79107875878161
 208.6253000000000 16.81485554209343
 209.7035000000000 16.77062433208757
 210.7817000000000 16.60245438476200
 211.8598000000000 16.77522983009107
 212.9380000000000 16.75611021512382
 214.0162000000000 16.80517721621971
 215.0943000000000 16.63210348859212
 216.1725000000000 16.67837069340520
 217.2507000000000 16.61155354097071
 218.3288000000000 16.45209510105235
 219.4070000000000 16.34708040295551
 220.4852000000000 16.21595280212958
 221.5633000000000 16.39291557004116
 222.6415000000000 16.42804054535265
 223.7197000000000 16.35449278881118
 224.7978000000000 16.24885397263904
 225.8760000000000 16.33625494830901
 226.9542000000000 16.38603003201388
 228.0323000000000 16.31459330789982
 229.1105000000000 16.10604290388566
 230.1887000000000 16.28993444817633
 231.2668000000000 16.31185750359679
```

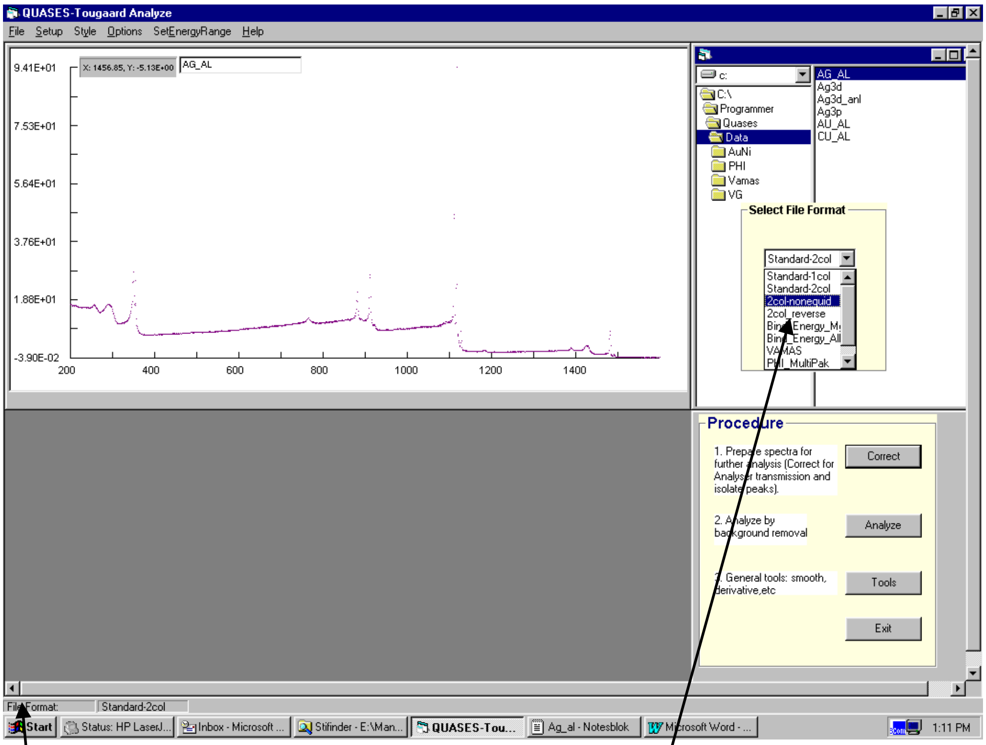
1. Prepare spectra for further analysis (Correct for Analyser transmission and isolate peaks).

2. Analyze by background removal

3. General tools: smooth, derivative,etc

File Format: Standard-2col

**Figure 6.1** Double click a file in the filelist to start the editor



1. Prepare spectra for further analysis (Correct for Analyser transmission and isolate peaks).

2. Analyze by background removal

3. General tools: smooth, derivative,etc

File Format: Standard-2col

**Figure 6.2**

Click here to change
data file format

Select new format

## File Formats.

QUASES accepts a range of different data file formats.

The data format can be changed by either

- click **FileFormat** in the lower left part of the screen

or

- click **Setup** in the menu bar

This opens the box **Select File Format** in the **Filelist** box.
Click the arrow next to the text box and get a list of possible file formats. (See fig. 6.2).

Select one of the file formats by clicking it.
The chosen file format appears in the in the lower left part of the screen (see fig.6.2)

## Standard-2col

This is the default data format used in QUASES.
The structure is:

```
Gold Au4d Sample # 205
@
366.4180   2.5168
366.8359   2.5122
367.2539   2.5266
367.6719   2.5116
368.0898   2.5200
368.5078   2.5124
368.9258   2.5348
369.3438   2.5287
369.7617   2.5142
```

The first several lines are comments while the data read by the programs start after the line following the character @.

The data are in columns where the first column is always the kinetic energy of the electrons and the second is intensities.

It is required that the increment in energy in the first column is the same for the whole data set. Use the data format **2col-nonequid** if the energy increment varies in the data set.

*Note that your data file must have a line with the character @ otherwise the file will not be read.*

## Standard-1col

The structure is:

```
"C:\Programmer\Quases\Data\AuNi\O50_anl with Class 1 profile and parameters 1 22 32.5 0 0 0 0 0 0 0 0 0 0 0 0 0 0"
"@"
323
1021.13
.500497
7.525895E-02
9.355836E-02
2.047564E-02
3.137738E-02
```

The first several lines are comments while the data read by the programs start after the line following the character @.

After that follows lines with:

the number of data points

the start energy Estart

the increment in energy EStep

intensity for energy Estart

intensity for energy Estart +EStep

intensity for energy Estart +2*Estep

intensity for energy Estart +3*EStep

etc

## 2col-nonequid

Use the data format **2col-nonequid** if the energy increment varies in the data set.
The structure is the same as for the format **2col-nonequid** except that the energy increment may vary in the data set.

## 2col-reverse

Use the data format **2col-reverse** if the energy is in two columns with energy and intensity with decreasing energies in the data set.

The structure is the same as for the format **Standard2col** except that the energies are decreasing rather than increasing.

The structure is:

```
"Put comments hereAnalysis of spectrum C:\Programmer\Quases\Data\AuNi\O46 with Class 1 profile and
parameters 1 22 32.5 0 0 0 0 0 0 0 0 0 0 0 0 0 0"
"@"
1182.791,7.077986E-05
1182.29,-6.630536E-03
1181.79,-8.209774E-03
1181.289,3.917136E-02
1180.789,-5.446143E-03
1180.288,3.796107E-03
```

## Bind_Energy_Mg

Use the data format **Bind_Energy_Mg** if the data are in two columns where the first column are the Binding energies and the second column the intensities and the spectrum has been recorded with Mg-Kα radiation.

The structure is:

```
"Put comments hereAnalysis of spectrum C:\Programmer\Quases\Data\AuNi\O46_anl with Class 1 profile
and parameters 1 22 32.5 0 0 0 0 0 0 0 0 0 0 0 0 0 0"
"@"
232.469995117187,7.525895E-02
231.969506835937,9.355836E-02
231.469018554687,2.047564E-02
230.968530273437,3.137738E-02
230.468041992187,.1067809
229.967553710937,7.930861E-02
229.467065429687,3.181648E-02
228.966577148437,2.196342E-02
```

## Bind_Energy_Al

Use the data format **Bind_Energy_Al** if the data are in two columns where the first column are the Binding energies and the second column the intensities and the spectrum has been recorded with Al-Kα radiation.

## VAMAS

Use the data format **VAMAS** if the data are in the standard VAMAS data format for a single energy range (multiple energy ranges are not supported).

### PHI-MultiPak

This data format is not supported in the current version.

### VG-Eclipse

This data format is not supported in the current version.

## Data format for the Analyzer response function.

In the program **Correct,** the analyzer transmission function may be specified in a file rather than by an exponent. The data format of the file that specifies the analyzer transmission function consists of comment lines and a line with the character @. After that follows two columns with data where the first column is the electron kinetic energy and the second column the corresponding relative transmission of the analyzer.

Usually it will be sufficient with data points for every 50 or 100 eV. The program Correct makes an interpolation between the points

The structure is:

```
@Trans100
200 1.699
250 1.641
300 1.553
350 1.463
400 1.376
450 1.300
500 1.233
550 1.171
600 1.116
650 1.066
700 1.017
800 0.943
900 0.877
1000 0.818
1100 0.768
1200 0.724
1300 0.687
1400 0.650
1500 0.620
```

## Data format when cross section is read from X-SECT

Usually one will use the Universal cross section or maybe one of the other standard cross sections supplied with QUASES (see Chapter 4 or 5). If however another cross section is applied, this must be contained in the file **X-Sect** in subdirectory **X-Sect**. The file format consists of comment lines and a line with the character @ after that follows two columns with data where the first column is the electron kinetic energy and the second column the corresponding product of the cross section and the inelastic mean free path.

The structure is:

```
Cross section
@
   2.000000E-01    2.434452E-04
   4.000000E-01    4.868194E-04
   6.000000E-01    7.300514E-04
   8.000000E-01    9.730702E-04
      1.000000    1.215805E-03
      1.200000    1.458185E-03
```

# *Chapter 7*

# 4. TOOLS

## 5. Smooth and Derivative

These programs are used to smooth or calculate the derivative of a spectrum.
It uses the Savitzky-Golay procedure.

Click **Tools**

Click **Smooth and Derivative** (see fig. 7.1).

Click the filename with the spectrum in the *Filelist* and get fig.7.2.

Both the unsmoothed and the smoothed spectra are plotted.

To increase the visibility of the plotted points, the point size may be changed by selecting **Style** from the menu bar, click **Linewidth**, click **Higher** to increase the point size, click **Lower** to decrease the point size.

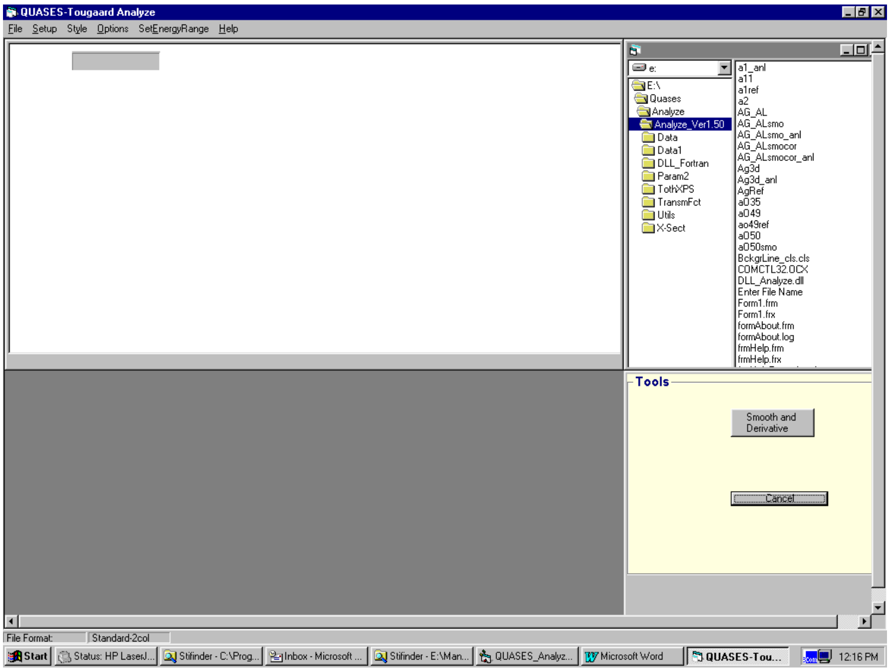
**To change the degree of smoothing** (see fig. 7.2 and 7.3):
change the values of
*6. Number of points*
*Order m of polynomial fit*

**To calculate the derivative of the spectrum**(see fig. 7.4 and 7.5):
Click option *Derivative*
Then change the parameters
*7. Number of points*
*Order m of polynomial fit*

**To save the smoothed or derivative spectrum:**
A default filename (original name with extension smo or drv) is automatically given. This name can be changed by clicking the textbox and typing a new name.

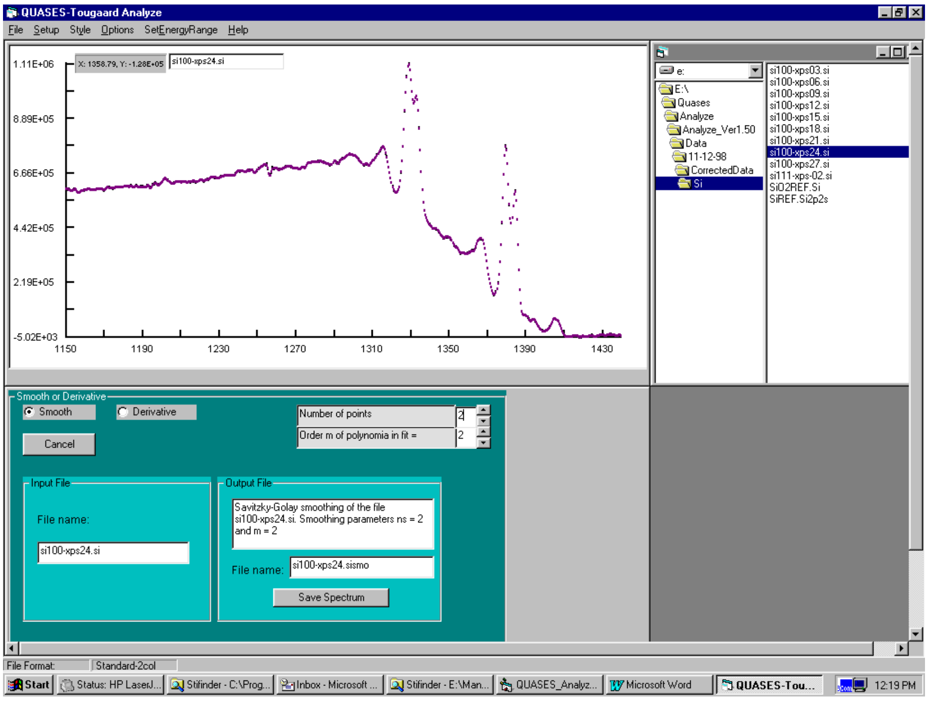
Click **Save Spectrum.**

The filename with the saved spectrum appears in the filelist box.



File Format: Standard-2col

**Figure 7.1**



● Smooth ○ Derivative

Number of points: 2

Order m of polynomia in fit = 2

Input File – File name: si100-xps24.si

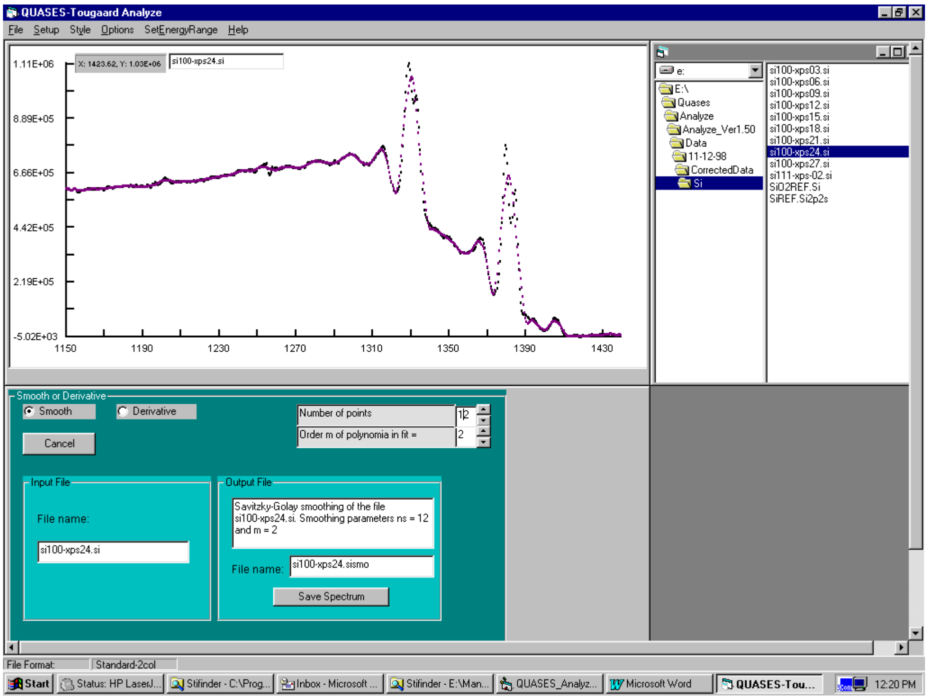
Output File:

Savitzky-Golay smoothing of the file si100-xps24.si. Smoothing parameters ns = 2 and m = 2

File name: si100-xps24.sismo

File Format: Standard-2col

**Figure 7.2** Click smooth to smooth a spectrum.



● Smooth ○ Derivative

Number of points 12

Order m of polynomia in fit = 2

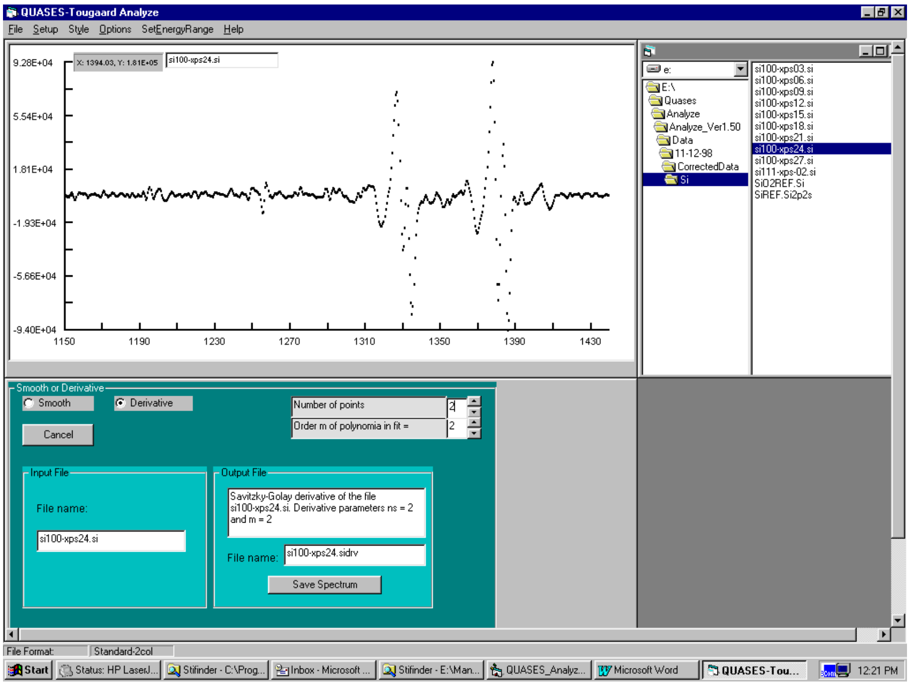
Input File – File name: si100-xps24.si

Output File: Savitzky-Golay smoothing of the file si100-xps24.si. Smoothing parameters ns = 12 and m = 2

File name: si100-xps24.sismo

File Format: Standard-2col

**Figure 7.3** The degree of smoothing is changed by changing the **Number of Points** and **Order m of polynomial fit.**



○ Smooth ● Derivative

Number of points 2

Order m of polynomia in fit = 2

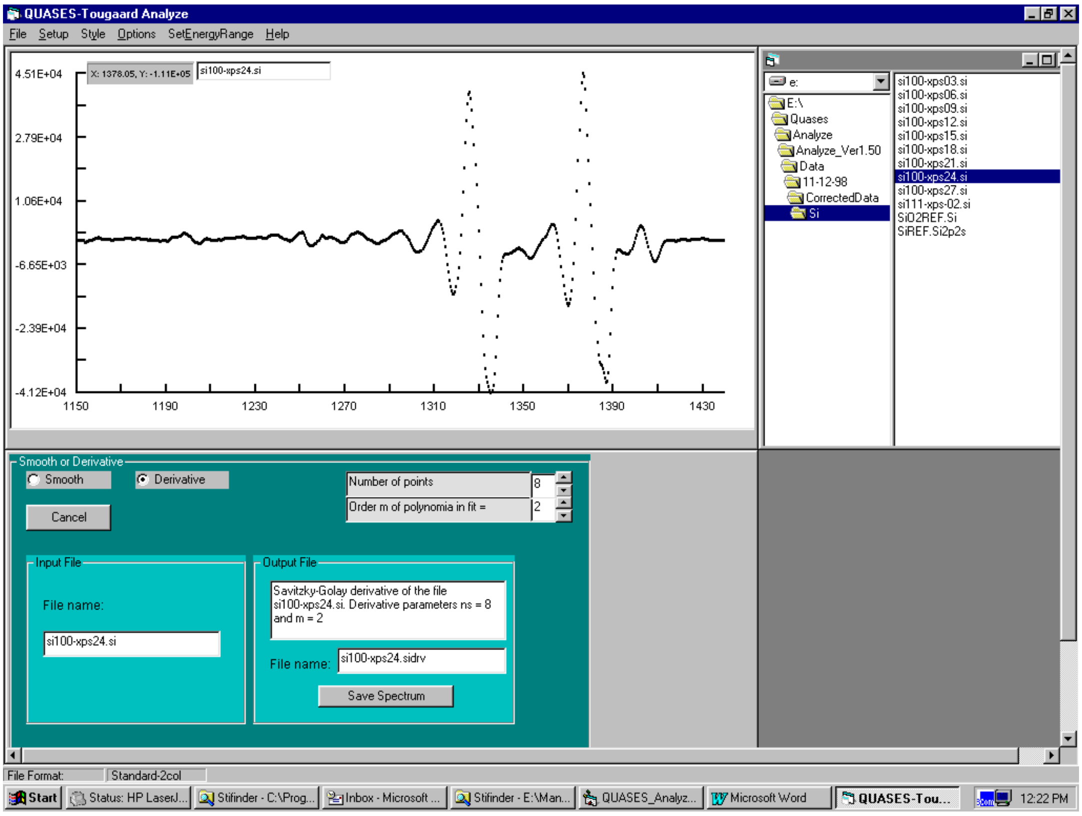
Input File – File name: si100-xps24.si

Output File: Savitzky-Golay derivative of the file si100-xps24.si. Derivative parameters ns = 2 and m = 2

File name: si100-xps24.sidrv

File Format: Standard-2col

**Figure 7.4** Click Derivative to differentiate the spectrum.



○ Smooth ● Derivative

Number of points: 8

Order m of polynomia in fit = 2

Input File — File name: si100-xps24.si

Output File: Savitzky-Golay derivative of the file si100-xps24.si. Derivative parameters ns = 8 and m = 2

File name: si100-xps24.sidrv

File Format: Standard-2col

**Figure 7.5** The degree of smoothing in the derivative spectrum is changed by changing the **Number of Points** and **Order m of polynomial fit.**

**QUASES-Tougaard**