User's Guide

QUASES-XS-REELS

**Quantitative Analysis of Surface Electron Spectra
Cross Sections determined by
Reflection Electron Energy Loss Spectroscopy**

Version 2.2

by

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**Software for Quantitative REELS
and Determination of Inelastic
Electron Scattering Cross Sections**

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0.   Introduction.

In the past, experimental methods to determine the inelastic scattering cross section for electrons moving in solids have largely relied on experiments where electrons passed through an extremely thin solid film [1]. Such experiments are however exceptionally difficult and for electron energies below ~ 10 keV such experiments can only be carried out for a few special solids.

A new experimental method to determine the effective inelastic electron scattering cross section was proposed some years ago [2-5]. In this new method, the inelastic electron scattering cross section is determined from analysis of the energy distribution of a mono-energetic beam of electrons that is reflected from a solid surface so-called Reflection Electron Energy Loss Spectroscopy (REELS). This is a very simple experiment that can be easily implemented for almost any solid or even for a nano-meter thin film on a substrate. Furthermore, the experimental facility is available in most surface analytical labs.

The inelastic electron scattering cross section gives valuable information on the electronic structure of the surface region of the solid. It is also an important quantity in the QUASES method for non-destructive analysis of the 3 dimensional nano-structure of surfaces by XPS and AES which was developed during the past years [6-9]. Using the QUEELS software package, it is also possible to determine the dielectric function and optical properties of thin films as well as the inelastic electron mean free path [16,17,18,19] from a simple analysis of the inelastic cross section. A software package QUEELS-$\varepsilon(k,\omega)$-REELS has been developed for this purpose (see www.quases.com)

Because of the importance of the inelastic electron scattering cross section, several research- and surface analysis institutes have expressed their interest in a user friendly software package that could make the algorithm for determination of the inelastic electron scattering cross section easily available.

To meet this demand, it was therefore decided to develop and market the software package QUASES™_XS_REELS (Quantitative Analysis of Surfaces by Electron Spectroscopy cross sections determined by REELS).

For further information please see

    www.quases.com

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Chapter 1

1. Concept of the QUASES™_ XS_REELS analysis procedure.

The theory behind QUASES_XS_REELS analysis is described in the publications [2-6] and outlined in Chapter 2 below. These papers also describe several experimental applications to various materials.

The QUASES-XS-REELS software package uses a REELS spectrum measured with primary electrons at energy E to determine the product $IMFP{\cdot}K(T)$ of the inelastic electron mean free path and the inelastic electron scattering cross section $K(T)$.

$K(T)dT$ is the probability that an electron of energy E shall loose energy in the range T, $T+dT$ per unit path length travelled in the medium.

Note that the output from QUASES_XS_REELS is in absolute units. The units are: $K(T)$ $[eV^{-1} \cdot Å^{-1}]$, $IMFP$ $[Å]$, and therefore $IMFP{\cdot}K(T)[$ $eV^{-1}]$. The integral

$$L\_KArea = \int_{0}^{E} IMFP K(T) dT \qquad\qquad 1.1$$

 is dimensionless. From the definition of the inelastic electron mean free path

$$IMFP = \frac{1}{\int_{0}^{E} K(T) dT} \qquad\qquad 1.2$$

Therefore we expect $L\_KArea \sim 1$. Because the measured energy loss range is smaller than $0 - E$ and because of weak effects of multiple elastic scattering events, we always expect $L\_KArea < 1$. In practice it is usually found to be in the range $0.7 < L\_KArea < 0.95$, where the lower values are found for $E \sim$ few hundred eV and the higher values at higher E. See [2-5].

1.1 Universality Classes of Inelastic electron scattering cross sections

It has been found that in many cases the overall behaviour of the cross section K(T) can be described with reasonable accuracy by Universal formulas valid for different classes of materials. This may be useful for parameterisation of the general shape of the cross sections found from analysis of REELS experiments with the QUASES_XS_REELS software package. In this section we will therefore briefly summarize the definition of these

Universality classes.

Depending on the class of materials, a function with either two, or three parameters is needed to describe the main characteristics of the cross sections of that class [4].

For most metals, their oxides and alloys, the *Universal cross section* [4]

$$\lambda_i(E)K(E,T) = \frac{BT}{\left(C + T^2\right)^2} \qquad 1.3$$

with $C = 1643\,\text{eV}^2$ and $B \cong 3000\,\text{eV}^2$ 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 [1] that the main characteristics of the cross section can be described by the *Three-parameter Universal cross section*

$$\lambda(E)K(E,T) = \frac{BT}{\left(C - T^2\right)^2 + DT^2} \qquad 1.4$$

where the three parameters B, C, and D have been determined for each class of materials (e.g. polymers, semiconductors, free-electron-like solids [4]).
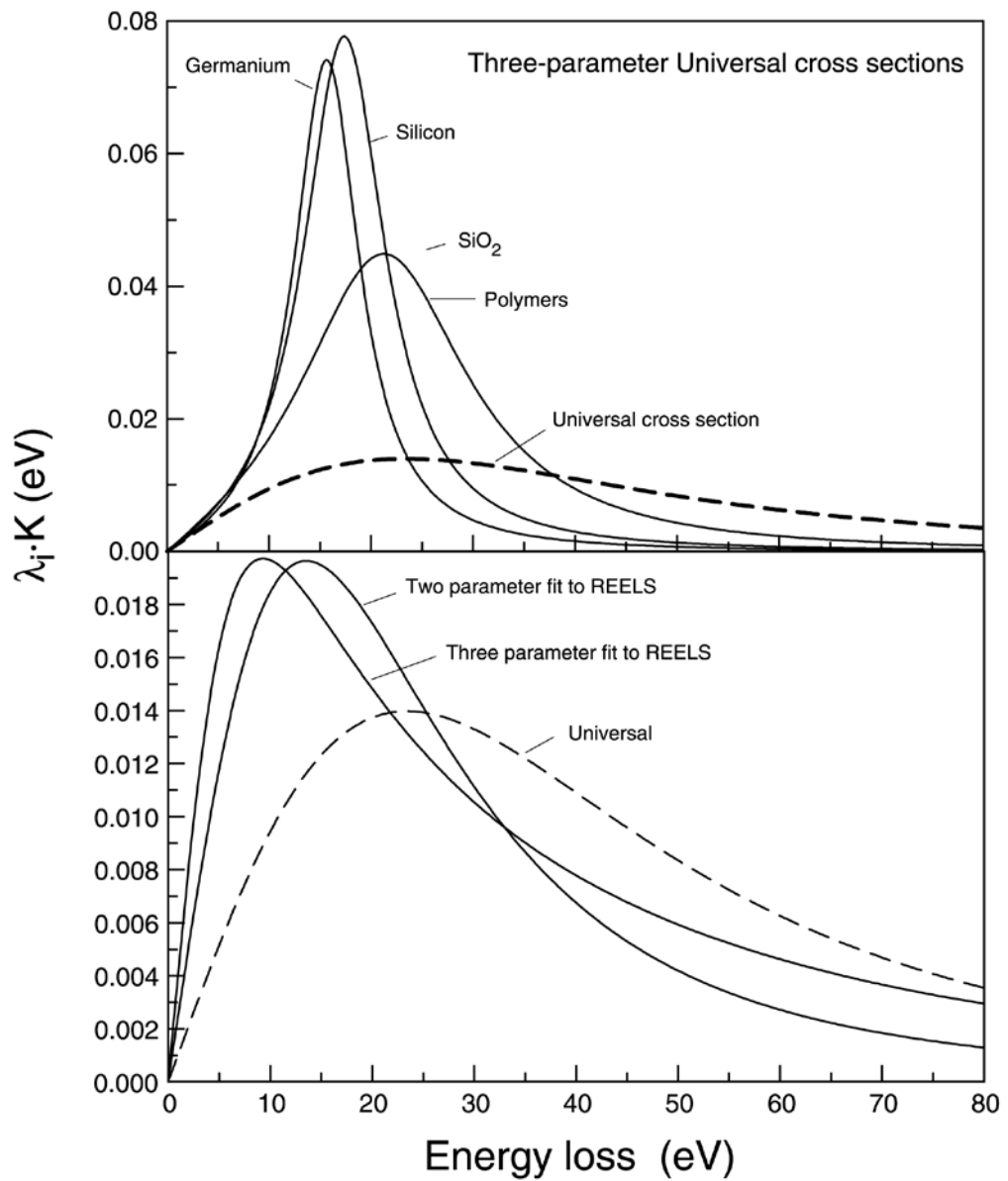
Figure 1.1 shows cross sections for various types of solids. The parameter values are given in table1. These cross sections are all included in the QUASES-Tougaard software (www.quases.com).

TABLE 1. Parameters for the Universal cross sections in eqs.(1.3) and (1.4). B^N is the value of B for which the cross section is normalized. Some of the cross sections are plotted in Fig. 1.1

Class of materials	$B\ [eV^2]$	$B^N\ [eV^2]$*	$C\ [eV^2]$	$D\ [eV^2]$
UNIVERSAL CROSS SECTION (EQ. 1.3)				
Metals and their oxides	2866	3286	1643	—
THREE – PARAMETER UNIVERSAL CROSS SECTION (EQ.1.4)				
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
*REELS CROSS-SECTION FOR TRANSITION METALS AND THEIR OXIDES**.*				
Fit to Universal Cross Section (eq 1.3)	760	1100	550	—
Fit to Three- parameter Universal Cross Section (eq.1.4)	4210	4645	1000	13300

* B^N is the value of B for which the cross section is normalized. Some of the cross sections are plotted in Figure 3.

** The REELS cross sections were determined from analysis by the QUASES-XS-REELS software of REELS spectra of Fe, Pd, Ti, Cu, Ag, and Au recorded at 2000 eV primary electron energy [5].

1.2   QUANTITATIVE REELS

In reflection electron energy loss spectroscopy (REELS), the solid surface is bombarded with a mono-energetic beam of electrons. These interact with the electrons in the surface region of the solid and the energy distribution of the backscattered electrons gives valuable information on the electronic structure and chemical bonds in the outermost few nano-meters [10,11]. By varying the primary energy of the electrons, the probing depth can be changed, and the relative importance of surface and bulk excitations can be varied [12,13]. More extensive quantitative applications of REELS were later made possible by using detailed models for electron-solid interactions [2,3 ,14,15]. These applications include the determination of cross sections for inelastic electron scattering [3,4], dielectric and optical properties of thin films [16,17,18], and the structure of thin films [19,20,21,22,23].

1.3   Algorithm for quantitative analysis of REELS.

Figure 1.2 shows a measured REELS spectrum and with the QUASES-XS-REELS software it is analyzed as follows. The spectrum is divided into channels $j(i)$ where $j(1)$ is the channel at the lowest energy and $j(i_p)$ the channel at the elastic peak energy. The energy separation between channels is E_{step}. The spectrum is then separated into the two spectra $j_{el}(i)$ consisting of the elastic electrons and $j_l(i)$ consisting of the inelastically scattered electrons. The energy range of the elastic peak is from E_{low} to E_{high} and the corresponding channels are i_{low} and i_{high} (see Figure 1.2).

Let $K(i)$ denote the probability for an electron with the elastic peak energy to lose energy $i \cdot E_{step}$ per unit energy loss and per unit path length traveled in the solid. The product of the inelastic electron mean free path and the inelastic electron scattering cross section $\lambda_i \cdot K(i)$ for energy loss $T = i \cdot E_{step}$ can then be calculated with the recursion formula [2,3, 25]
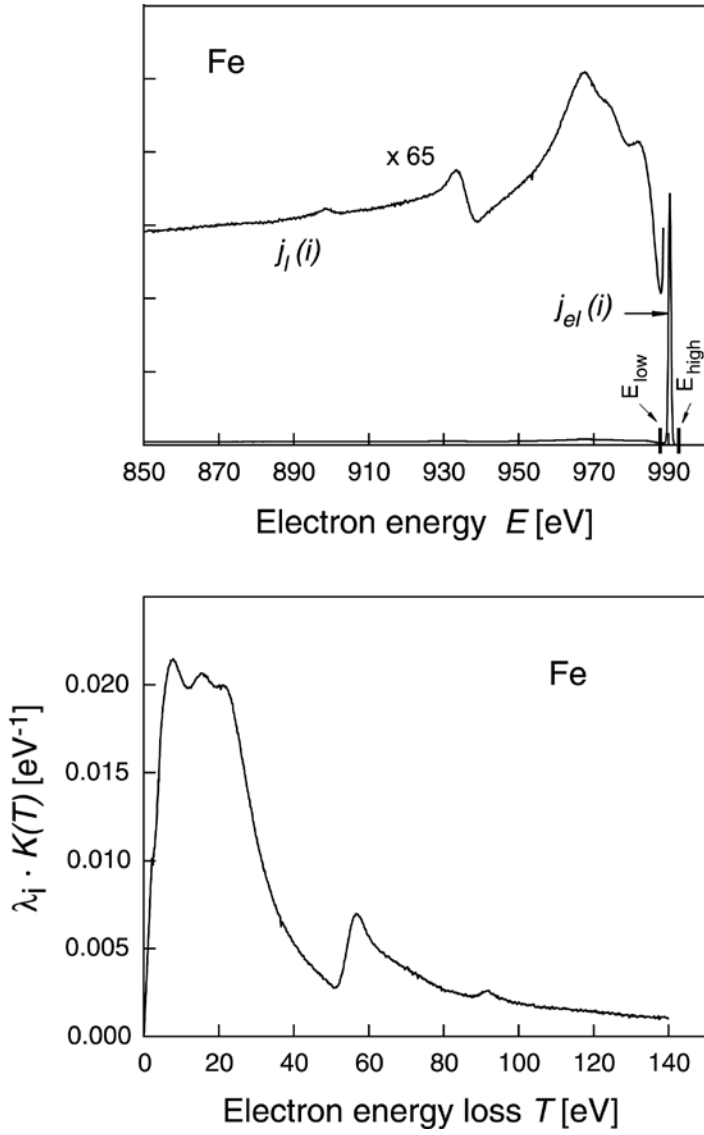
Figure 1.2 Quantitative analysis, by eqs.1.5-1.7 of a REELS spectrum from Fe.

$$\lambda_i \cdot K(0) = 0 \qquad\qquad 1.5$$

and for $n = 1$, i_p

$$\lambda_i \cdot K(n) = \frac{j_l(i_p - n) - \sum_{m=1}^{n-1} \lambda_i \cdot K(n-m) \cdot j_l(i_p - m) \cdot E_{step}}{A_p} \qquad 1.6$$

where A_p is the area of the elastic peak:

$$A_p = \sum_{i=ilow}^{ihigh} j_{el}(i) \cdot E_{step} \qquad\qquad 1.7$$

This determines $\lambda_i K(E,T)$ in the energy loss range $T = 0$ to $T = i_p\, E_{step}$.

1.4 Applications in quantitative surface analysis

Figure 1.2, shows the REELS spectrum from an Fe foil obtained with a 990 eV primary electron beam [4]. The measured spectrum contains intensity from electrons that have lost energy in multiple inelastic scatterings. Also shown is the single scattering cross section $\lambda_i \cdot K(T)$ determined from eqs. 1.6.

Since multiple scattering features are removed, in the $\lambda_i \cdot K(T)$ curve, it is easier to interpret structure and to extract chemical bonding information. Because $\lambda_i \cdot K(T)$ is in absolute units, it is also possible to compare the $\lambda_i \cdot K(T)$ spectra on an absolute scale and quantitative information on both electronic excitations and on thin film growth can be obtained. For example, it has been shown that the nano-structure of particles on substrates can de found by fitting the determined $\lambda_i \cdot K(T)$ to a linear combination of $\lambda_i \cdot K(T)$ from the substrate and the surface atoms [20,21,22]. By application of a realistic model [14,15] for description of the effective $\lambda_i \cdot K(T)$ in terms of the dielectric function of the thin film, it is also possible to determine the dielectric function and optical properties of thin films as well as the inelastic electron mean free path [16,17,18,19]. This can be done with the software package QUEELS-ε(k,ω)-REELS (see www.quases.com).
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Chapter 2

2. Installing and Running QUASES_XS_REELS

System Requirements

- A PC with running Microsoft Windows.

- A CD-ROM disk drive for installing QUASES_XS_REELS.

- A hard disk with 10 MB free disk space.

- VGA graphics 800x600 (1024x768 or better is recommended).

- A mouse

2.1　Installing QUASES_XS_REELS

1. Insert the compact disc in the CD-ROM drive.

2. Open the directory **Install QUASES_XS_REELS**

3. Click **Setup**.
   This starts installation of **QUASES-XS_REELS**. Follow the instructions on the screen.

Note: The program assumes 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.

Chapter 3

3. QUASES_XS_REELS analysis.

In a REELS spectrum, the difference between the intensity at the elastic peak and the inelastic background is usually very large (see fig. 3.1) when the experimental settings are selected to give a high count rate in the region of the inelastic scattered electrons the count rate in the energy region of the elastic peak gets very high. This can result in saturation of the spectrometer in the energy region of the elastic peak. To avoid this, it is therefore often an advantage to record the spectrum in two parts: the elastic peak region and the inelastic peak region. A single spectrum is then constructed from these two spectra. The QUASES_XS_REELS program package has facilities to handle this (see fig. 3.2). In this chapter it is described which method should be used depending on how the spectra were recorded.
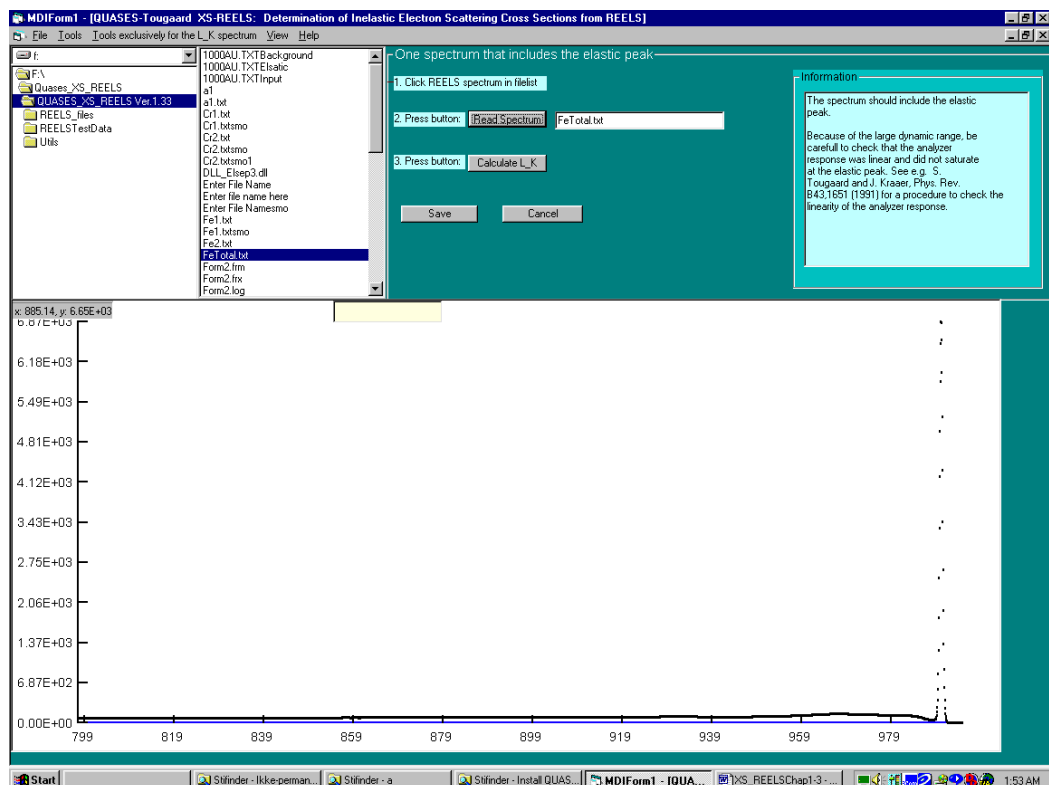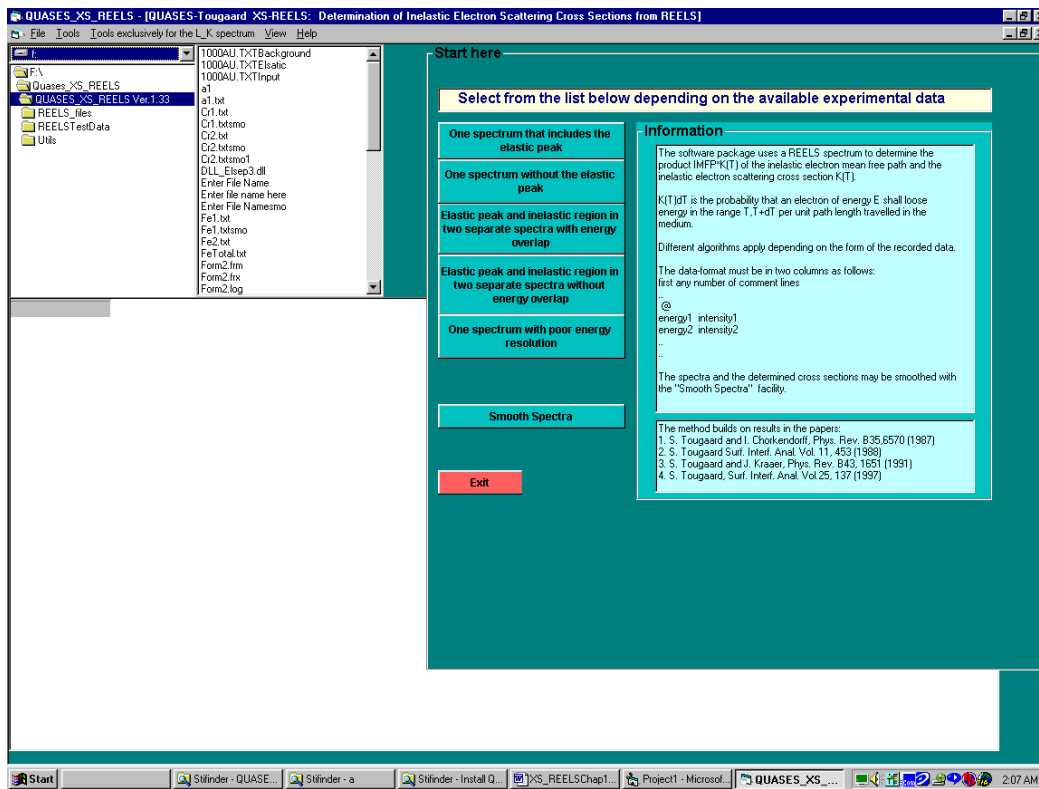

Figure.3.1 REELS spectrum from Fe.

Figure 3.2 QUASES_XS_REELS opening menu.

3.1   One Spectrum that Includes the Elastic Peak

Here the spectrum is recorded over the full energy range and it includes the elastic peak. Because of the large dynamic range in the REELS spectrum (see fig. 3.1), it is important that one is careful to check that the analyzer response was linear and did not saturate in the energy region of the elastic peak. See S. Tougaard and J. Kraaer, Phys. Rev. B43,1651 (1991) for an experimental procedure to check the linearity of the analyzer response. Since QUASES_XS_REELS is a quantitative analysis program such deviations are important for a correct interpretation of the data.
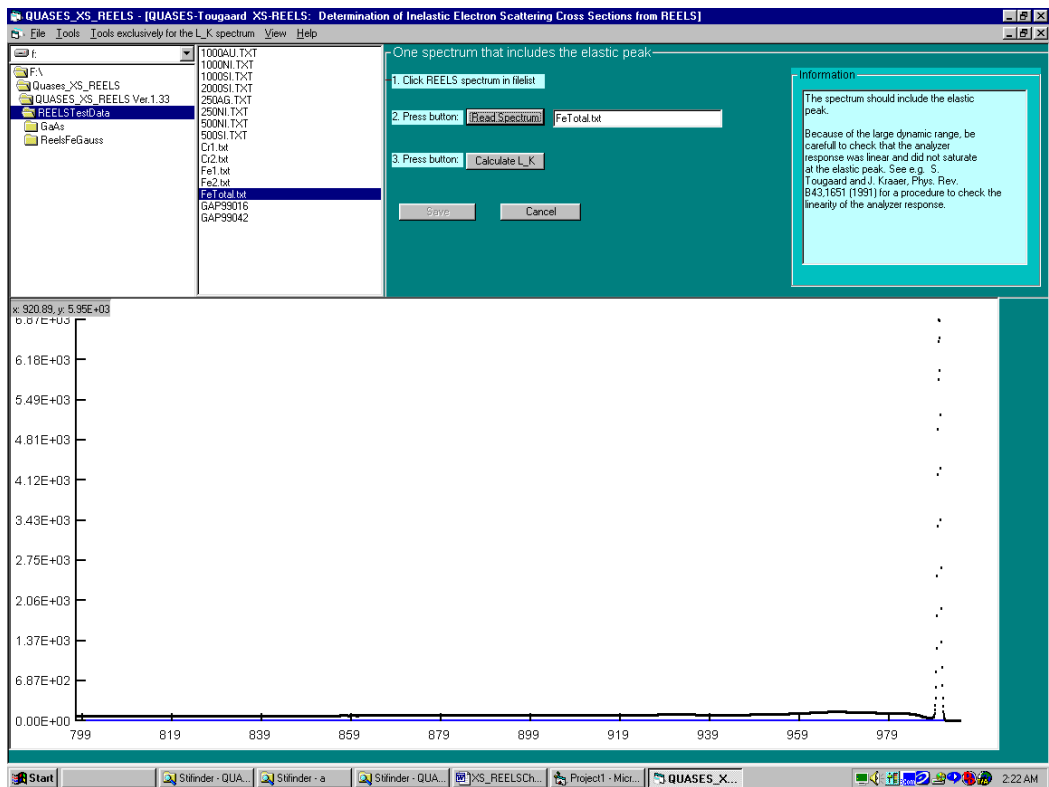
Figure 3.3

3.1.1 Tutorial Example:

Analysis of REELS from Fe.
Spectrum needed: FeTotal.txt

1. Click: *One Spectrum that Includes the Elastic Peak* (see Fig. 3.2)

2. Find the file with the REELS spectrum using the file manager in the right left part of the screen.

3. Click the filename (FeTotal.txt).

4. Click *Read Spectrum* and get Fig. 3.3

5. Click *Calculate L_K* and get Fig. 3.4. This is the determined *IMFP·K(T)* function in the absolute units [eV^{-1}].

6. To save the determined IMFP· K(T) function:

   a. Click *Save*
   b. Change the text in the text box if you wish. This text is saved in the file together with the data.
   c. Type a file name in the *File Name* text box.
   d. Click *Save Cross Section*. See fig. 3.5
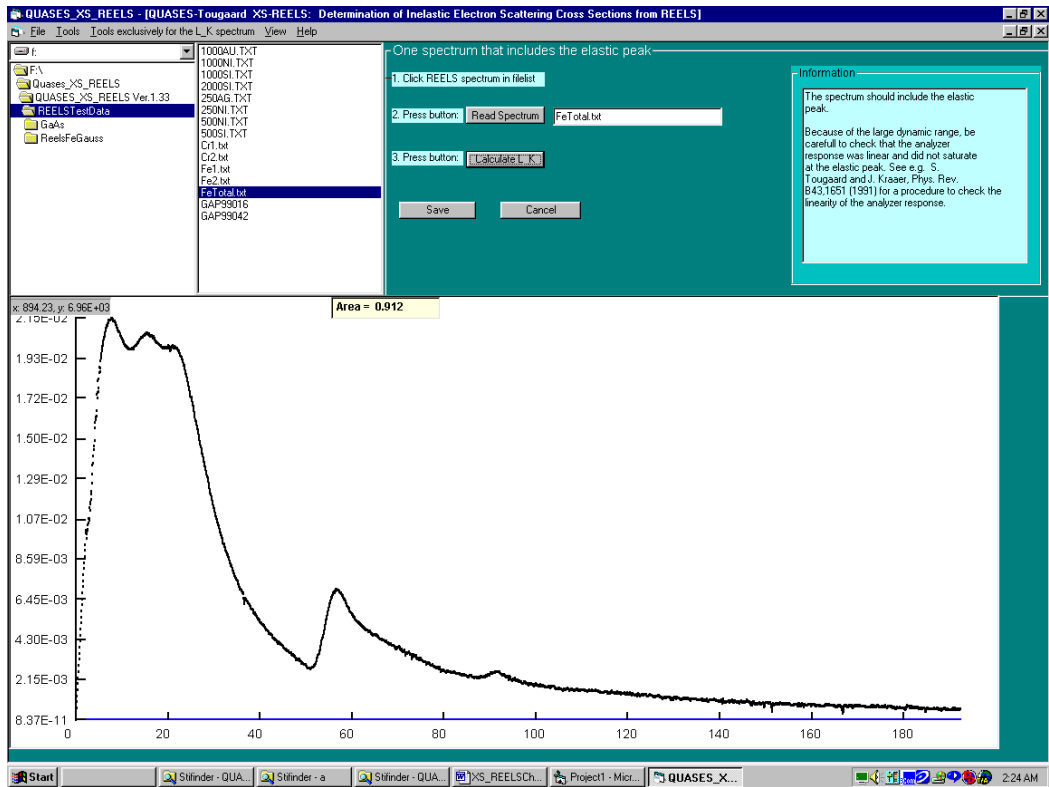   e. The new file is saved and the filename appears in the filelist box.

Figure. 3.4 Determined cross section. Note that the ordinate is *IMFP·K(T)* in the absolute unit eV^{-1}.
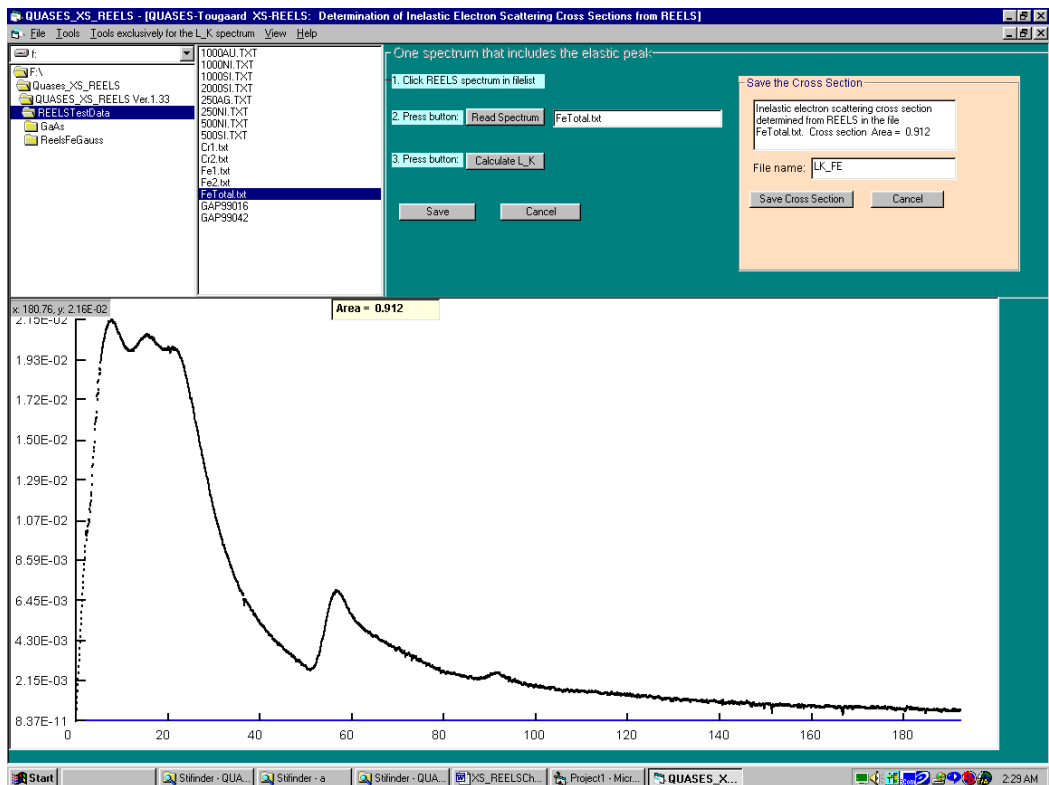

Figure. 3.5

3.2 One Spectrum without the Elastic Peak

This menu applies to the situation where the spectrum is only recorded over the energy range of the inelastically scattered electrons, for example from 1 eV below the energy of the primary electrons.

This removes the possible problem of saturation in the response of the analyzer in the region of the elastic peak mentioned above. There are two things that are not quantitatively included in the spectrum in this case:

1. the relative intensity of the primary electron beam

2. the exact energy of the primary electrons.

Since QUASES_XS_REELS is a quantitative analysis program, this information is therefore supplied during the analysis procedure (see the tutorial example below).

3.2.1 Tutorial Example:

Analysis of REELS from Fe.
Spectrum needed: Fe2.txt

1. Click: *One Spectrum without the Elastic Peak* (see Fig. 3.2)

2. Find the file with the REELS spectrum using the file manager in the right left part of the screen.

3. Click the filename (Fe2.txt).

4. Click *Read Inelastic* and get Fig. 3.6

5. Click *Calculate L_K* and get Fig. 3.7. This is the determined *IMFP·K(T)* function in the absolute units $[eV^{-1}]$.

6. Adjust the value in the "Adjust LK Area" text box. (This is needed because the elastic peak was not included in the measured spectrum). Select a value in the range ~ 0.7 – 0.95. Adjust for example the value of "LK_Area" until the cross section is non-negative for all values of the energy loss. Use a sufficiently high value so you observe that IMFP· K(T) approaches zero for large energy loss T.

7. Adjust the value of the elastic peak energy to the known value (the value you set for the electron gun beam energy)

8. To save the determined IMFP· K(T) function:

   a. Click *Save*
   b. Change the text in the text box if you wish. This text is saved in the file together with the data.
   c. Type a file name in the *File Name* text box.
   d. Click *Save Cross Section*. See fig. 3.5
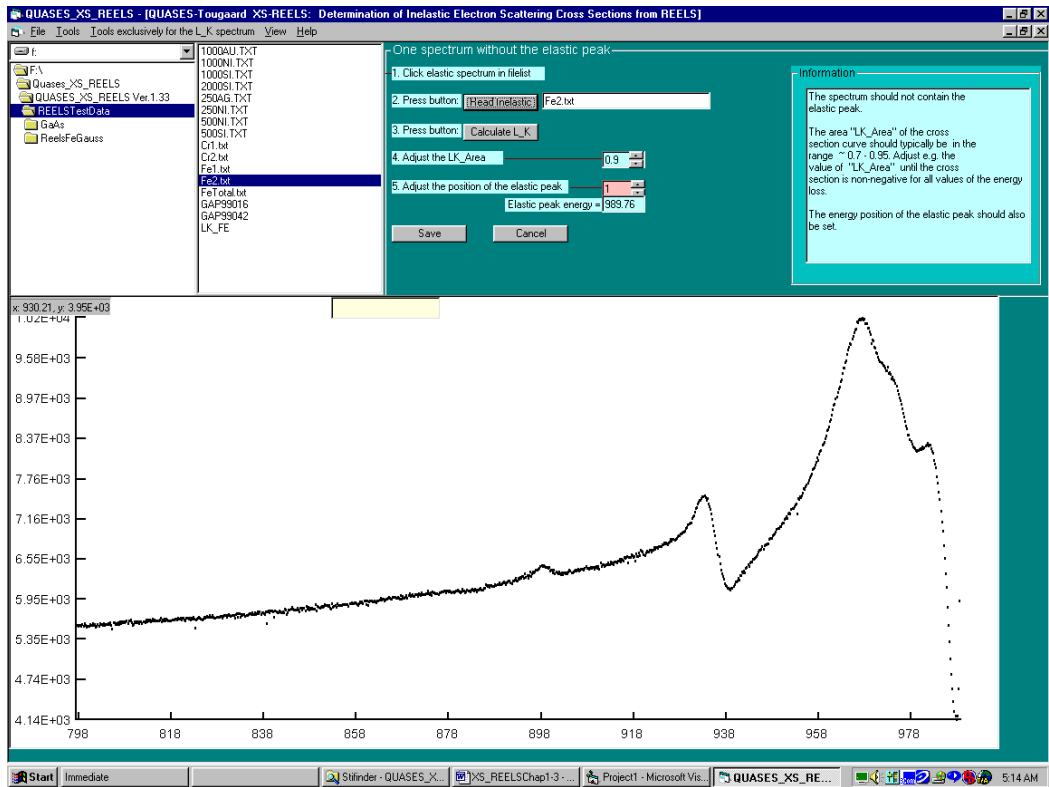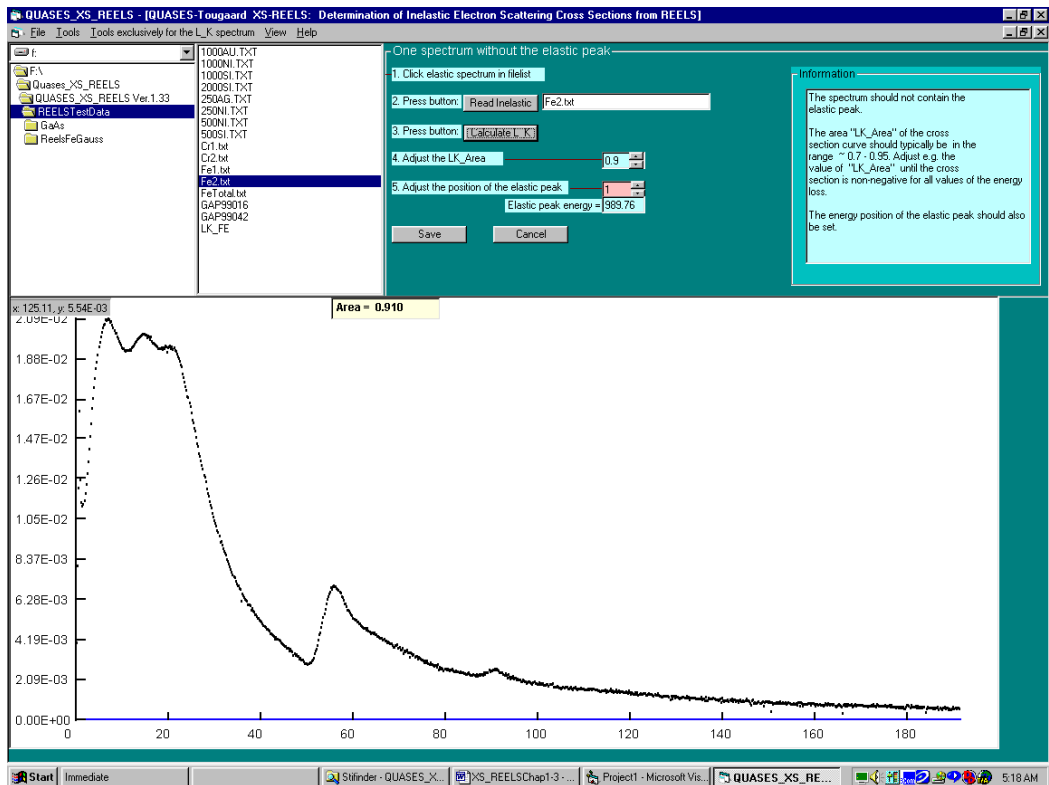   e. The new file is saved and the filename appears in the filelist box.
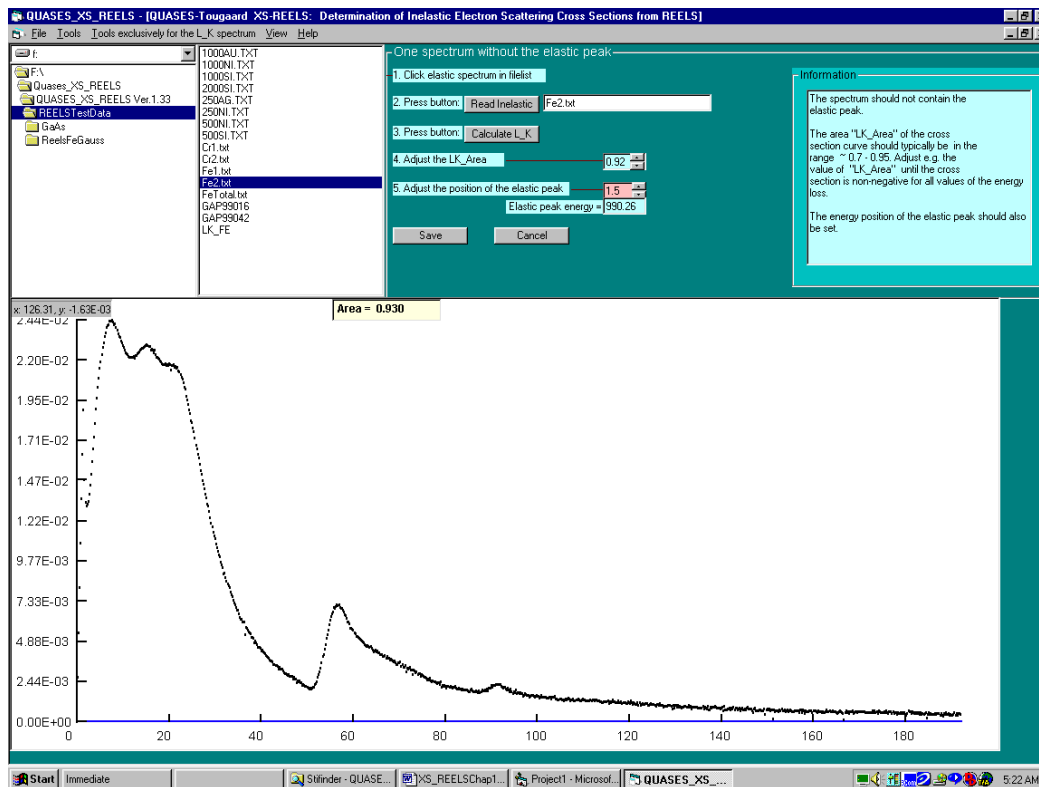
Figure 3.6

Figure 3.7

Figure 3.8

3.3   Elastic and Inelastic Region in Two Separate Spectra with Energy Overlap

This menu applies to the situation where the spectrum is recorded as two separate spectra: one with the elastic peak and one with the energy region of the inelastically scattered electrons. The two spectra should have a common energy range from *En1* to *En2*. The area in this energy range is used to normalize the intensities of the two spectra. The relative intensity of the two spectra needs therefore not to be known.

The reason that you would want to use record the two separate spectra is that it can be an advantage to apply a high electron current and a higher analyser pass energy when you record the energy region with inelastically scattered electrons since this will give an improved signal to noise level. You should note that when you use a higher electron gun filament current (to get higher emission), the beam energy is likely to increase by maybe 0.1-0.2 eV so you would want to correct for that. The elastic peak can however not be recorded with very high electron current and pass energy because the analyser is then likely to saturate. You will therefore record the elastic peak with lower beam current and maybe also lower pass energy.

The energy loss *Es* separates the regions where the intensity in the elastic and inelastic spectra are used. *Es* should be adjusted until the calculated cross section appears as a smooth function at the energy loss *Es*.

The energy grid in the two spectra need not be the same. The energy grid in the calculated cross section will be the same as that in the spectrum with the elastic peak.

3.3.1 Tutorial Example:

Analysis of REELS from Cr.
Spectra needed: Cr1.txt and Cr2.txt

1. Click: *Elastic and Inelastic Region in Two Separate Spectra with Energy Overlap* (see Fig. 3.2)

2. With the file-manager, find the file (Cr1.txt) with the REELS spectrum that includes the elastic peak.

3. Click the filename.

4. Click *Read Elastic* and get Fig. 3.9.

5. Find the file (Cr2.txt) with the REELS spectrum of the inelastic part.

6. Click the filename.

7. Click *Read Inelastic* and get Fig. 3.10

9. Click *Calculate L_K* and get Fig. 3.11. This is the determined *IMFP·K(T)* function in the absolute units $[eV^{-1}]$.

8. Adjust the value of Es with the up-down button until you get a smooth cross section and get fig. 3.12 (with Es=6 in this case)

9. Adjust the value of the elastic peak energy

10. To save the determined IMFP· K(T) function:

    a. Click *Save*
    b. Change the text in the text box if you wish. This text is saved in the file together with the data.
    c. Type a file name in the *File Name* text box.
    d. Click *Save Cross Section*. See fig. 3.5
    e. The new file is saved and the filename appears in the filelist box.

11. To plot and/or save the spectrum which is formed by the programme and that is used to calculate the cross section:
    a. Select from the menu bar: *View + Plot Intermedia Spectra* . See fig. 3.13
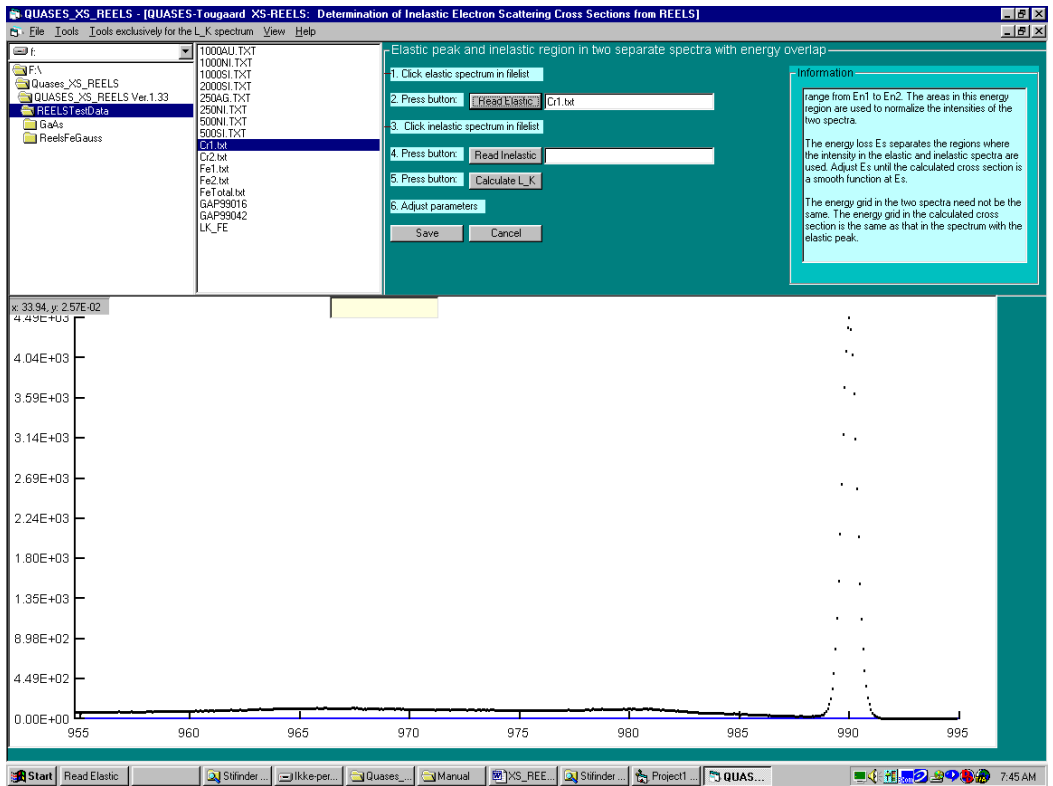   b. Plot and save the various spectra as indicated in the menu on fig. 3.13
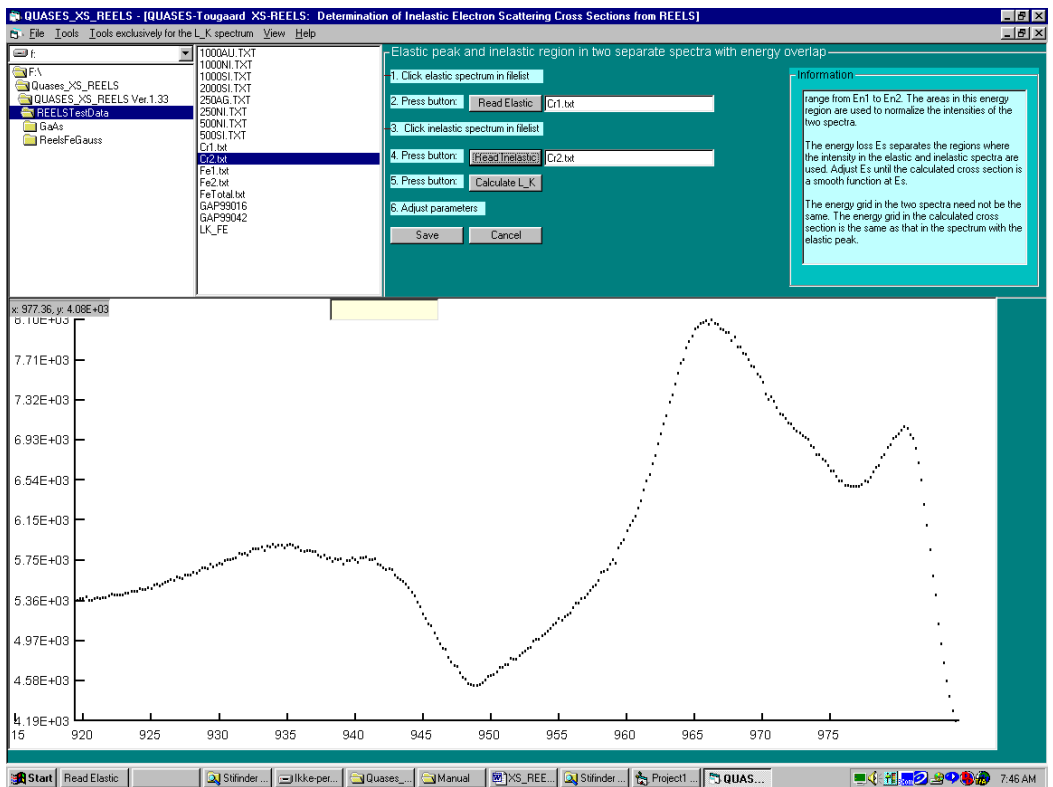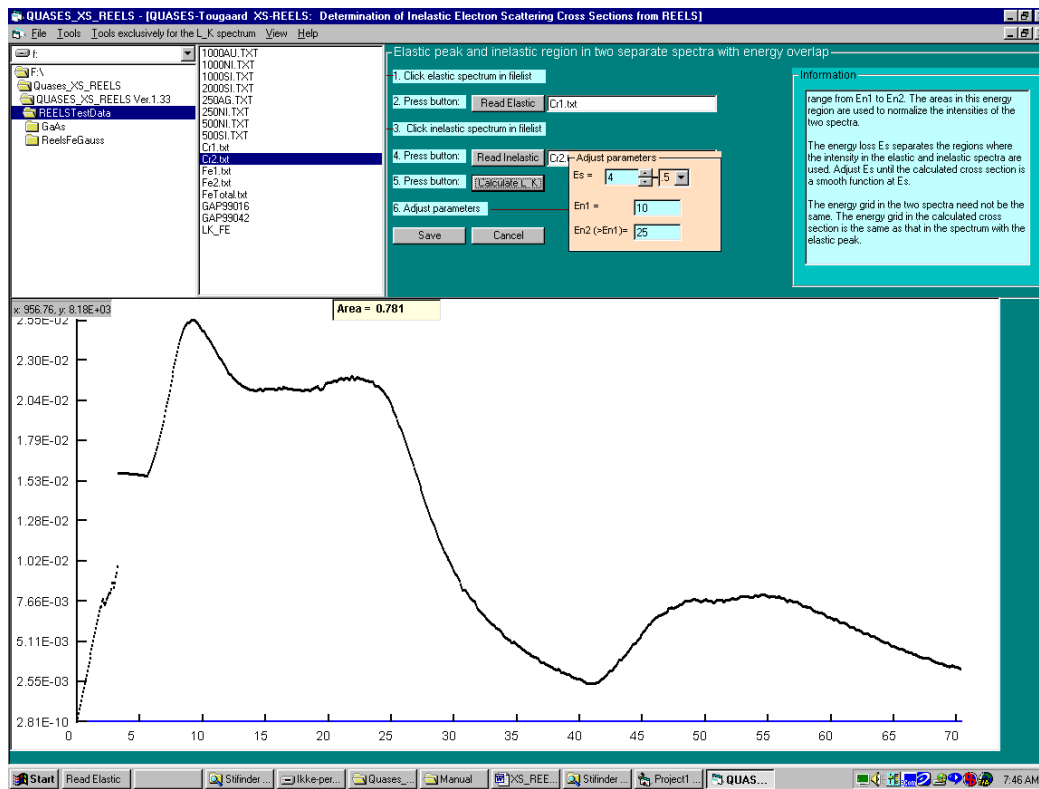
Figure 3.9
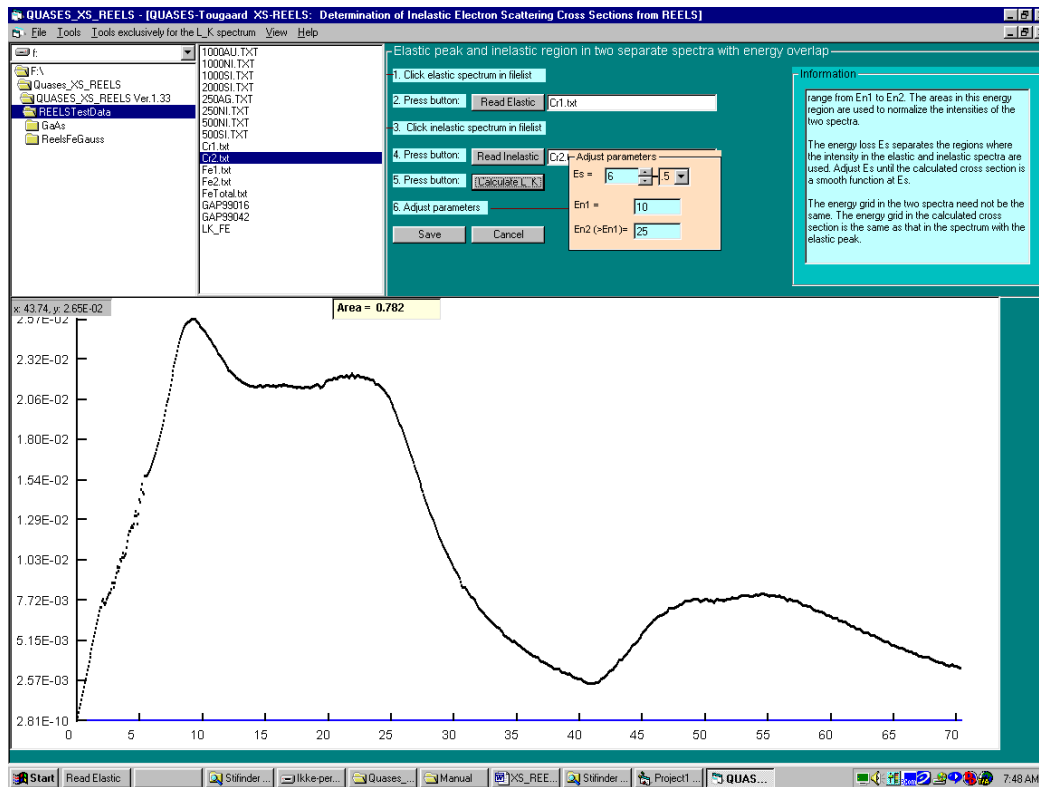
Figure 3.10

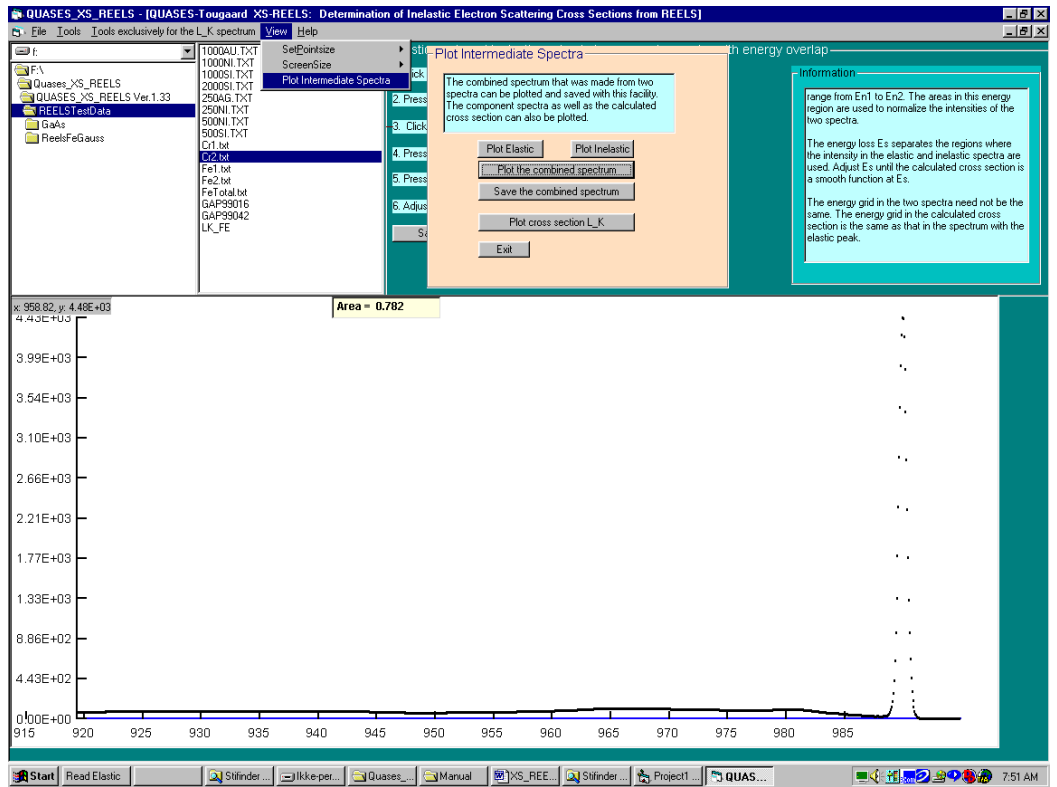**Figure 3.11**

Figure 3.12

Figure 3.13

3.4   Elastic and Inelastic Region in Two Separate Spectra without Energy Overlap

This menu applies to the situation where the spectrum is recorded as two separate spectra: one with the elastic peak and one with the energy region of the inelastically scattered electrons. The two spectra may have but need not have an overlapping energy range.

The intensity in the two spectra is normalized manually by visual inspection of the transition region between the two spectra on the plotted spectrum.

The energy grid in the two spectra need not be the same. The energy grid in the calculated cross section will be the same as that in the spectrum with the elastic peak.

3.4.1 Tutorial Example:

Analysis of REELS from Cr.
Spectra needed: Cr1.txt and Cr2.txt

1. Click: *Elastic and Inelastic Region in Two Separate Spectra without Energy Overlap* (see Fig. 3.2)

2. With the file-manager, find the file (Cr01.txt) with the REELS spectrum that includes the elastic peak.

3. Click the filename.

4. Click *Read Elastic* and get fig. 3.14.

5. Find the file (Cr2.txt) with the REELS spectrum of the inelastic part.

6. Click the filename.

7. Click *Read Inelastic* and get Fig. 3.15

8. Click *Adjust Factor* and get fig. 3.16

9. Adjust the value in the box *Multiply Elastic spectr by factor* until there is a smooth transition between the two spectra (see fig. 3.17).

10. Click *Calculate L_K* and get Fig. 3.18. This is the determined *IMFP·K(T)* function in the absolute units [eV^{-1}]

11. To save the determined IMFP· K(T) function:

    a. Click *Save*
    b. Change the text in the text box if you wish. This text is saved in the file together with the data.
    c. Type a file name in the *File Name* text box.
    d. Click *Save Cross Section*. See fig. 3.5
    e. The new file is saved and the filename appears in the filelist box.

12. To plot and/or save the spectrum which is formed by the programme and that is used to calculate the cross section:
    a. Select from the menu bar: *View + Plot Intermedia Spectra* . See fig. 3.13
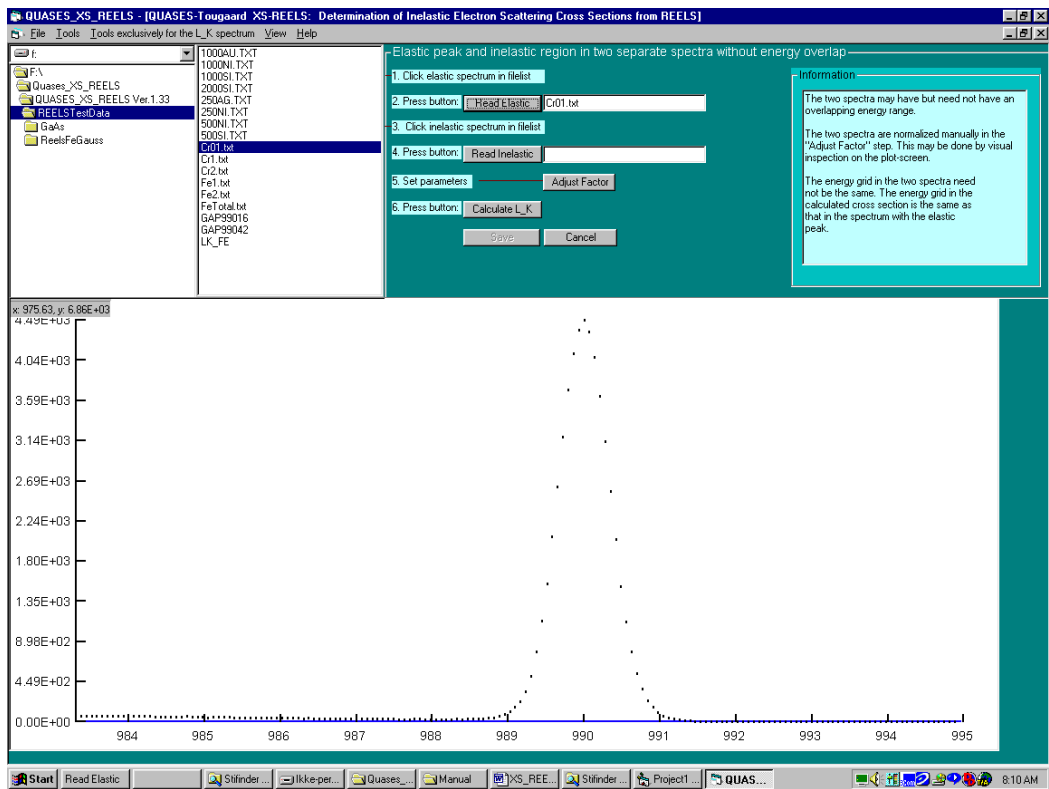   b. Plot and save the various spectra as indicated in the menu on fig. 3.13
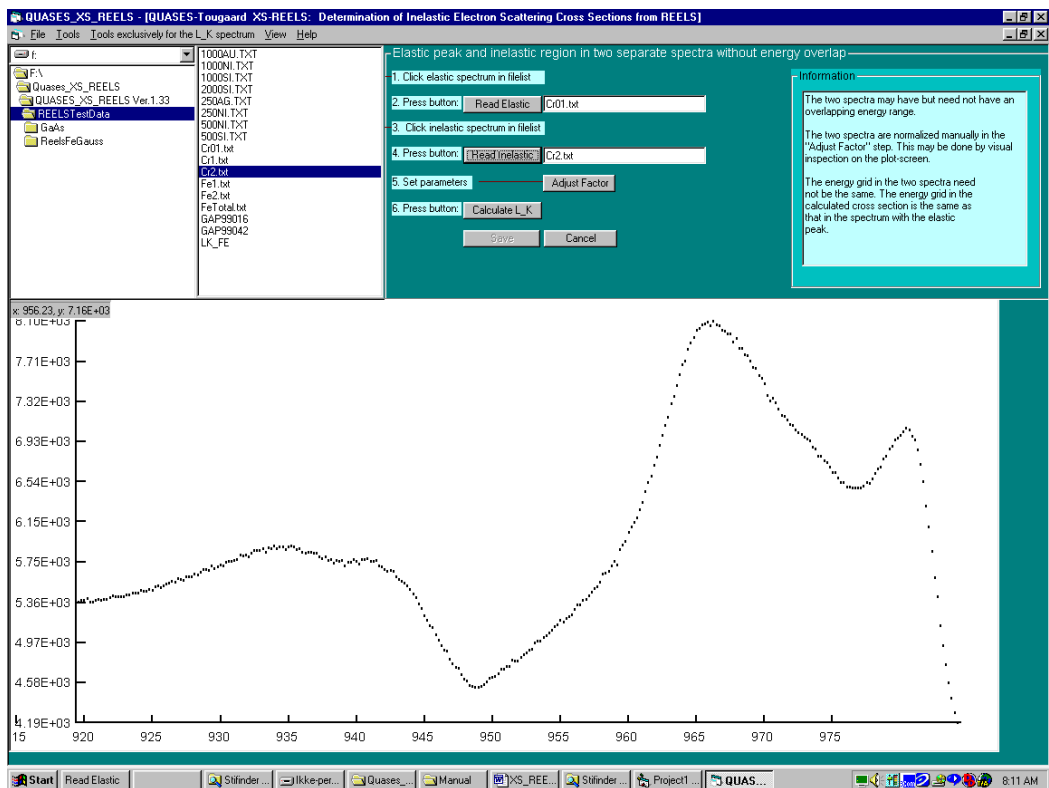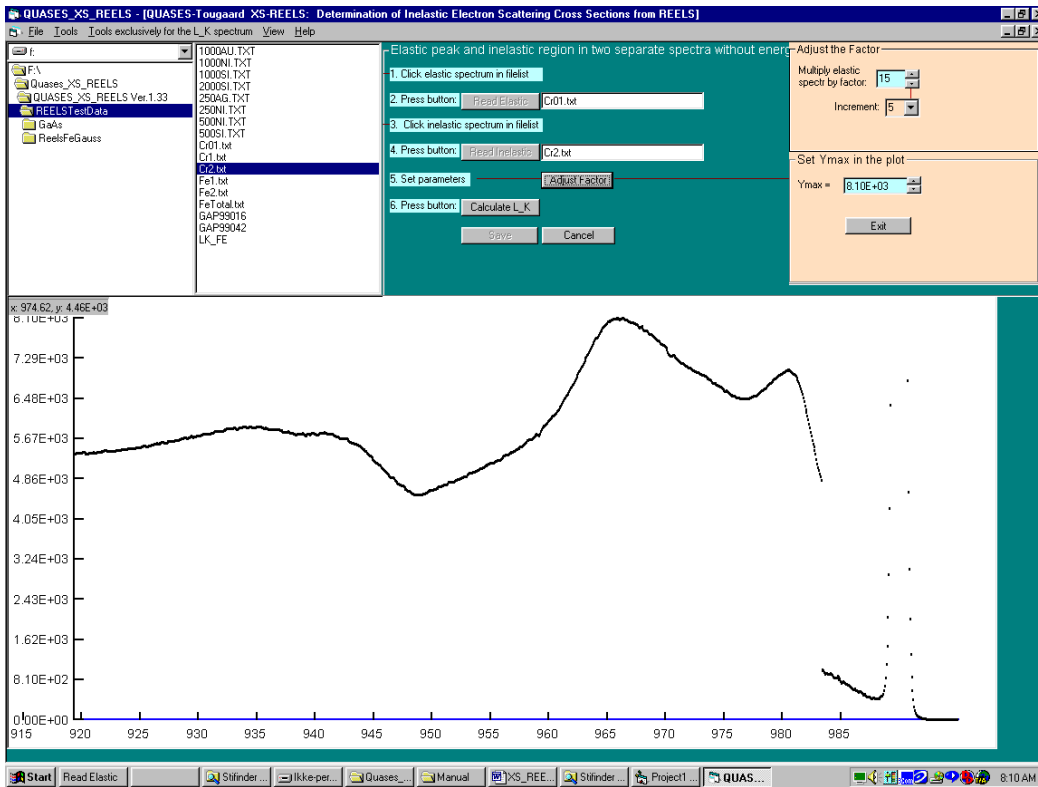
Figure 3.14
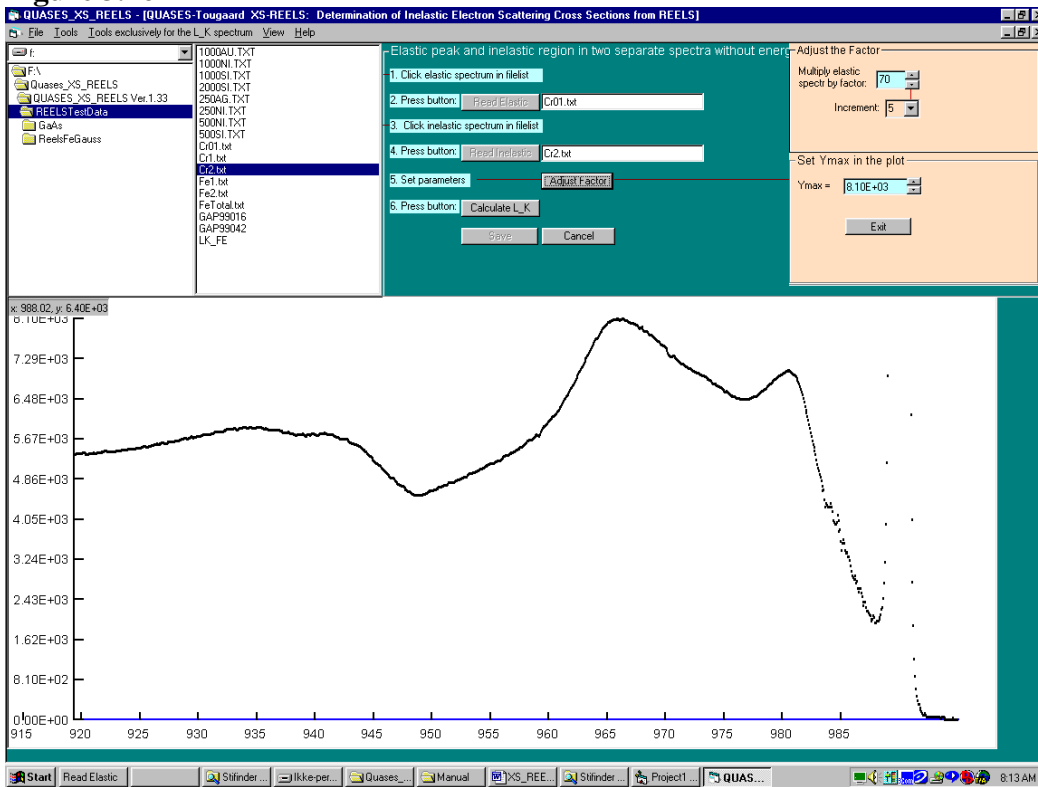

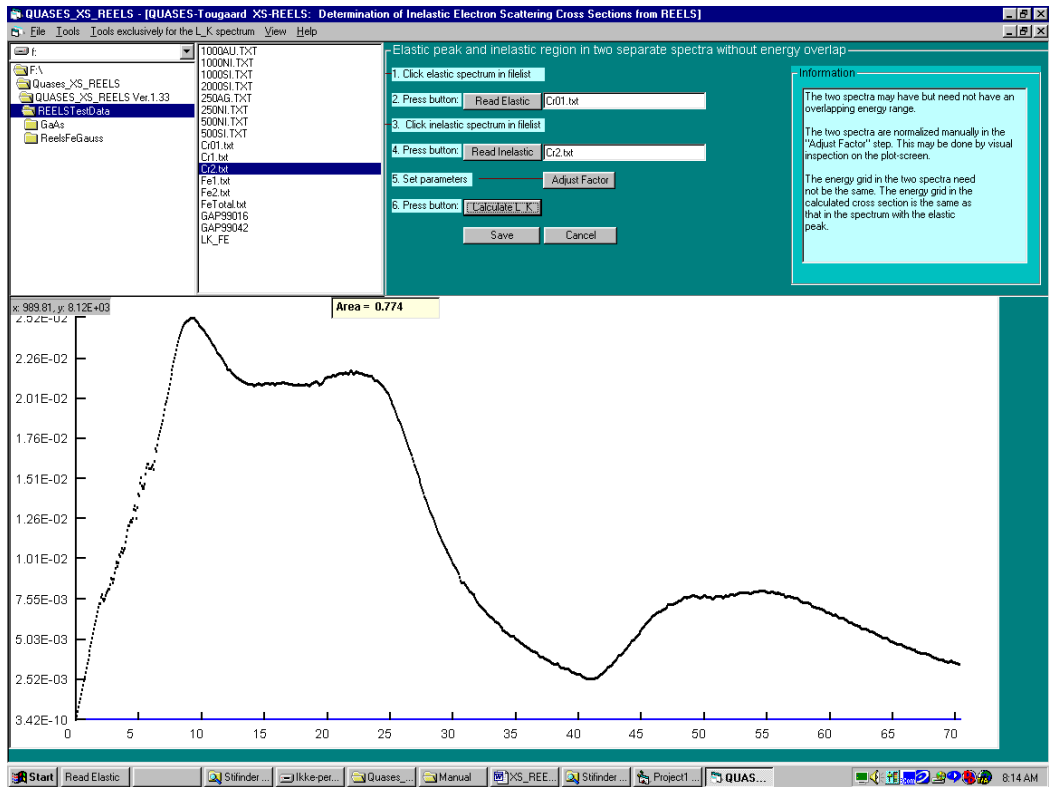**Figure 3.15**

Figure 3.16

Figure 3.17

Figure 3.18

3.5   One Spectrum with poor energy resolution.

Here the spectrum is recorded over the full energy range and it includes the elastic peak. In contrast to the situation in Sec. 3.1, the REELS spectrum is here recorded with a spectrometer with poor energy resolution (worse than ~2 eV). The elastic peak and the inelastic peak overlap strongly in energy.

The algorithm *ELPSEP* is used to separate the spectrum in an elastic peak spectrum and an energy loss spectrum (details of the *ELPSEP* algorithm are described in the paper: S. Tougaard, Surf. Sci. 464, 233 (2000).

Both the area and the energy position of the elastic peak are used when the cross section is calculated from the energy loss spectrum.

3.5.1 Tutorial Example:

Analysis of REELS from Si.
Spectrum needed: 1000Si.txt

1. Click: *One Spectrum with Poor Energy Resolution* (see Fig. 3.2)

2. Find the file with the REELS spectrum using the file manager in the right left part of the screen.

3. Click the filename (1000Si.txt).

4. Click *Read Spectrum* and get Fig. 3.20

5. Click *Calculate L_K* and get Fig. 3.21. This is the determined *IMFP·K(T)* function in the absolute units $[eV^{-1}]$

6. You may change the *discrimination level.* This is used to define the extension of the elastic peak. (See the paper: S. Tougaard, Surf. Sci. <u>464</u>, 233 (2000)).

7. You may also change the *linear region.* This is the energy loss region where the cross section is assumed to be linear.

8. To save the determined IMFP· K(T) function:

    a. Click *Save*
    b. Change the text in the text box if you wish. This text is saved in the file together with the data.
    c. Type a file name in the *File Name* text box.
    d. Click *Save Cross Section*. See fig. 3.5
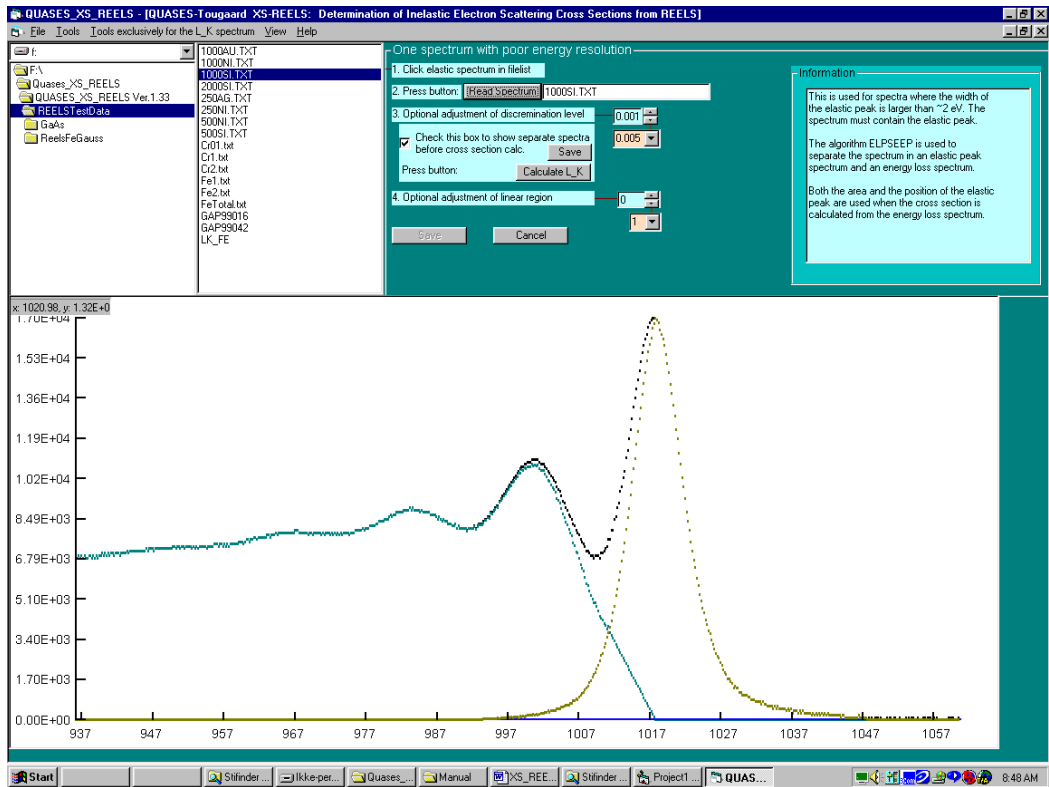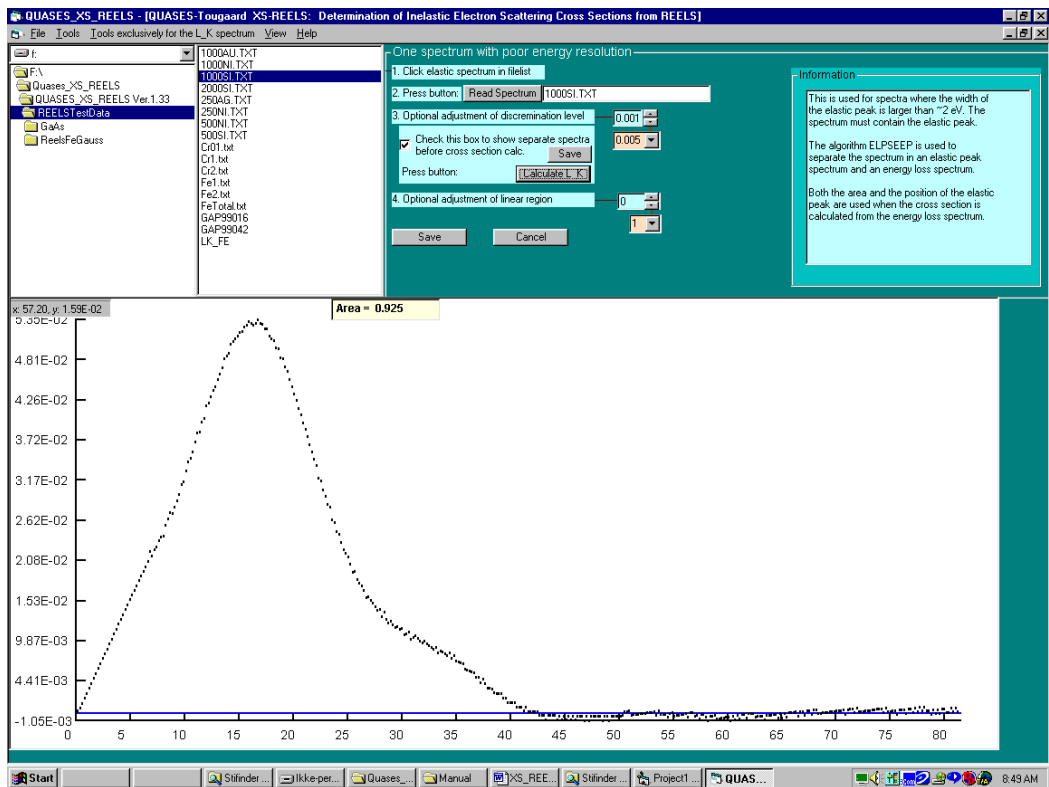   e. The new file is saved and the filename appears in the filelist box.

Figure 3.20

Figure 3.21

Chapter 4

4.   File Formats and File Management

It is helpful to be able to keep track of the experimental data files as well as of the files created by the programs.

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 data format.

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

On left hand side of the **Main Menu** is the **File Manager** (see fig. 3.1). 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 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.

File Formats.

QUASES_XS_REELS accepts a simple data file format.

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 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.

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

Note also: The program assumes 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.

Chapter 5

5.   Smooth.

This program is used to smooth a spectrum.
It uses the Savitzky-Golay procedure.

Click **Smooth Spectra** (see fig. 5.1).

Click the filename with the spectrum (Cr2.txt) in the *Filelist* and get fig.5.2.

Both the unsmoothed and the smoothed spectra may be plotted by clicking the check box. Use this to check the degradation in the spectral structure with increasing smoothening.

To increase the visibility of the plotted points, the point size may be changed by selecting *View* from the menu bar, click *SetPointSize*, click *Increase* or *Decrease* to increase or decrease the point size.

To change the degree of smoothing (see fig. 7.2 and 7.3):
        change the values of

Number of points ns
and

Order m of polynomial fit

To save the smoothed or derivative spectrum:
A default filename (original name with extension smo) 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.

Tutorial example. Smooth

1. Smooth Cr1.txt with ns = 4 and m = 2.
2. Save as Cr1.txtsmo
3. Smooth Cr2.txt with ns = 4 and m = 2.
4. Save as Cr2.txtsmo
5. Apply the option *Elastic Peak and inelastic region in two separate spectra with energy overlap* to determine the cross section from the files: Cr1.txtsmo and Cr2.txtsmo. You should get the spectrum in fig. 5.3.
6. Determine the cross section with the unsmoothed spectra Cr1.txt and Cr2.txt.You should get the cross section in fig. 5.4.
7. Compare the noise level in the two cross sections.

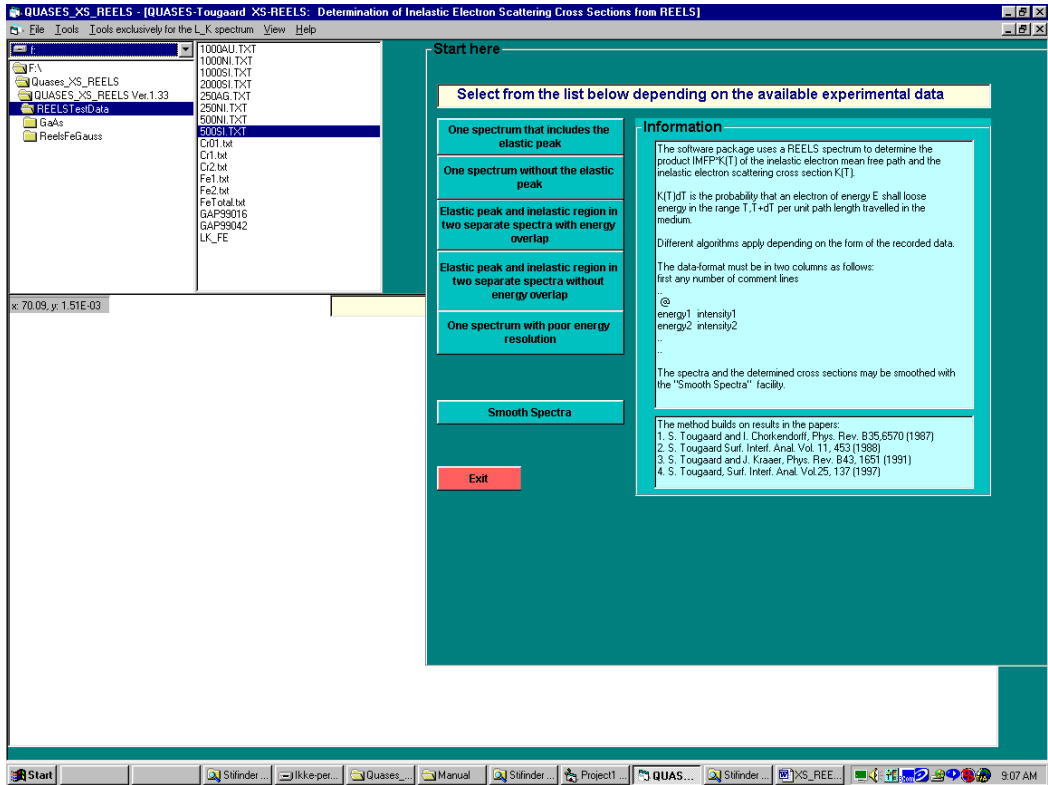The smooth facility may also be applied to smooth the cross section after it has been determined.
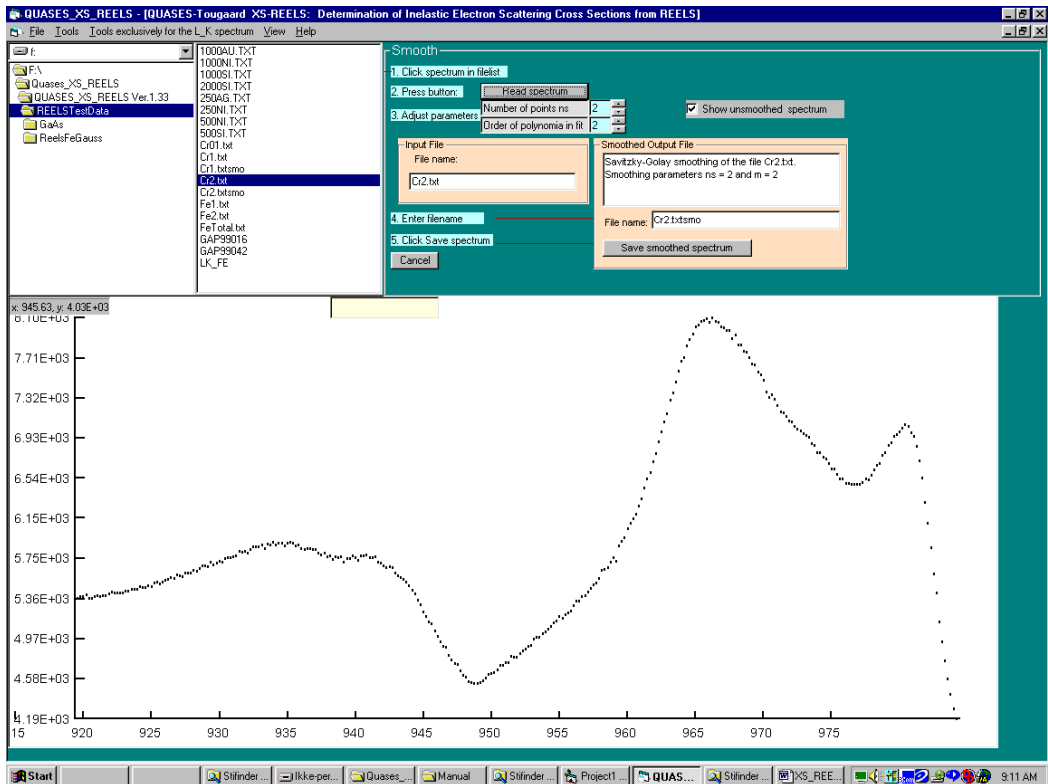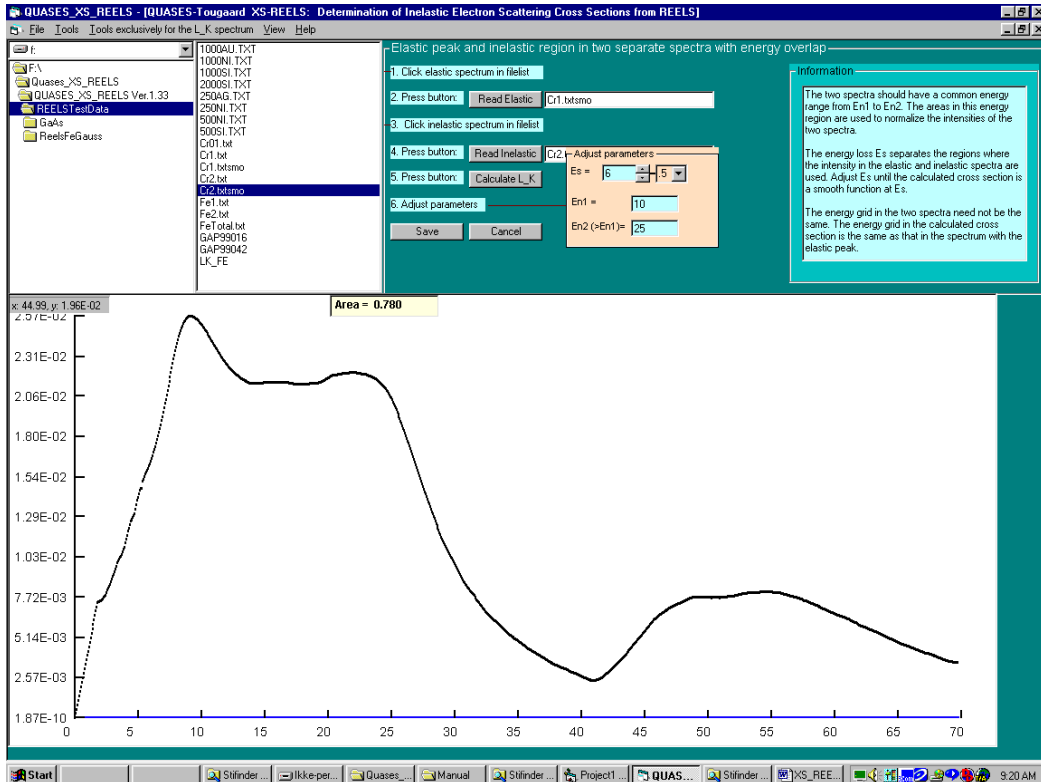
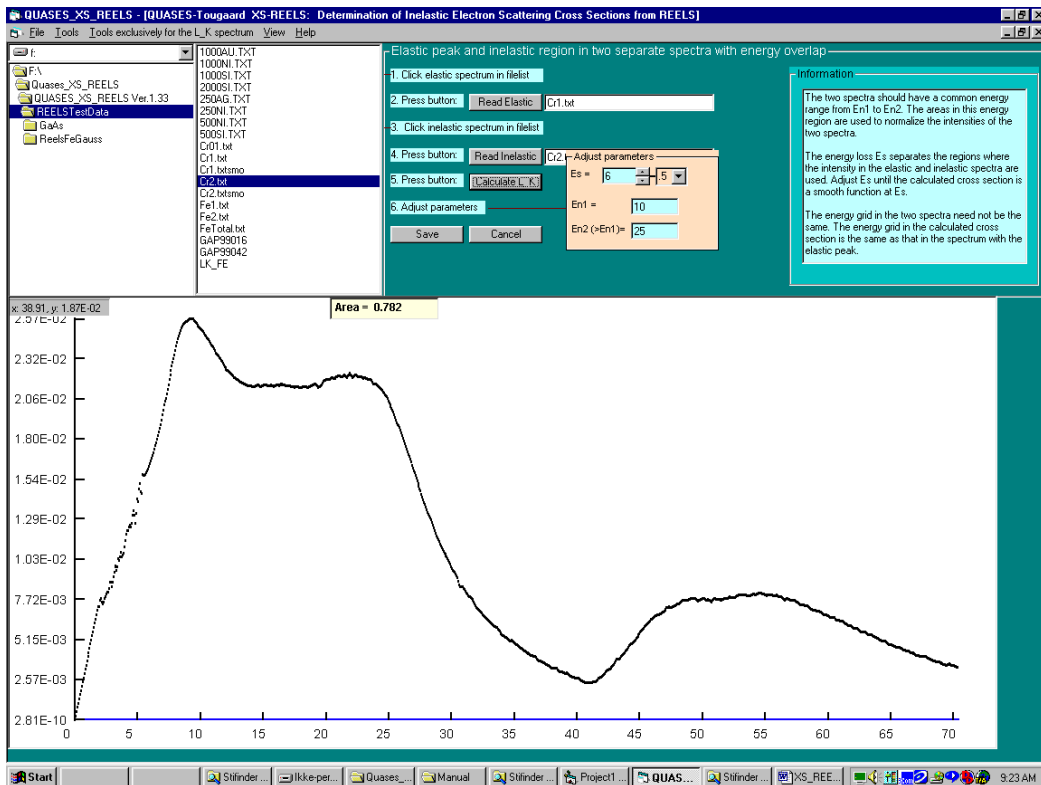**Figure 5.1**

Figure 5.2

Figure 5.3.

Figure 5.4

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