

User's Guide

QUEELS - $\varepsilon(k, \omega)$ - REELS

Software to determine the Dielectric and optical properties of thin films from REELS.

**Version 4.3
(including direct/indirect gap options)**

by

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**Software for Quantitative
Calculation of Inelastic
Electron Scattering Cross Sections
and determination of the dielectric function
from REELS experiments**

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Agreement for use of the software:

You are not allowed to use the software unless you have a license.

The software builds on the results published in:

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S. Tougaard and J. Kraaer, Phys. Rev. B43, 1651 (1991)

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1. Introduction

To control the functionality of new nano-technological structures it is important to be able to understand their electronic and optical properties. The basics of many of these properties can be described by the complex physical processes which take place when a charged particle moves in them and interact with the electrons in the solid. [1,2,3,4,5,6,7]. Models to describe this are also important for quantitative understanding of surface analysis techniques based on the interpretation of electron spectra such as X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES), transmission electron spectroscopy (TEELS) and reflection electron energy loss spectroscopy (REELS). These are influenced by the inelastic scattering processes that take place when an electron moves in the region near a solid surface. The actual energy losses depend on the particular experimental situation. Thus, an electron is attracted by its image charge when it is moving in the vacuum. It will therefore lose energy even after it has left the surface and similarly, an electron that moves in vacuum towards the solid surface gains energy. Likewise, the scattering properties for an electron moving close to the surface are different from that of an electron moving in the bulk of the solid. In photoemission and Auger experiments the effect of the static hole will also affect the scattering probabilities of the electron in the first few Å as it moves away from the point of excitation. These effects will also cause the “effective” inelastic mean free path to depend on the position of the electron with respect to the surface and with respect to the point of excitation.

We have been involved [3,5,6] in the development of semi-classical models based on a dielectric response description of the interaction between the moving electron and the electrons in the solids. In a first model we considered simplified expressions for the surface electron energy losses where it was assumed that the shape of the surface loss does not depend on the kinetic energy or the surface crossing direction and thus in this model the total excitation was expressed as a linear combination of surface $[\text{Im}(-1/(\epsilon+1))]$ and bulk $[\text{Im}(-1/\epsilon)]$ terms. It was however found that the coupling between surface and bulk excitations cannot be described with this model [F. Yubero and S. Tougaard , Surf Interf, Anal 19, 269 (1992)].

It is therefore necessary to use a much more elaborate model to get reliable quantitative information from low energy electron loss spectra [5,6]. The expressions are complicated and involve several infinite integrations and this has been a main hindrance for widespread practical use of the results. With the purpose of making the calculations available to the general community, we decided in 2001 to start development of user friendly and practical software packages. The present manual and software package is the first in a series of such packages. Other software packages like QUEELS-XPS deals with energy loss in photo electron and Auger spectra and QUEELS-Surface Loss with energy loss in thin films in general (see www.quases.com for updated information).

The theory and several experimental tests on the validity of the theory were performed together with co-workers over the past decade. The tests showed that the theory is of good validity [8,9,10 ,11,12, 13] even for electron energies of ~ 100 eV. The model gives basic fundamental knowledge on the excitation properties of solids and it allows e.g. also to determine the dispersion in wavevector dependence of the dielectric function.

The theory has been applied to determine the dielectric function and the optical properties of solids and thin films over a large range of energy loss [8-31] and for theoretical calculations of the importance of surface excitations [32,37]. From the dielectric function, one can calculate important optical properties like the refractive index and the extinction and absorption coefficient as well as the inelastic mean free path for electrons.

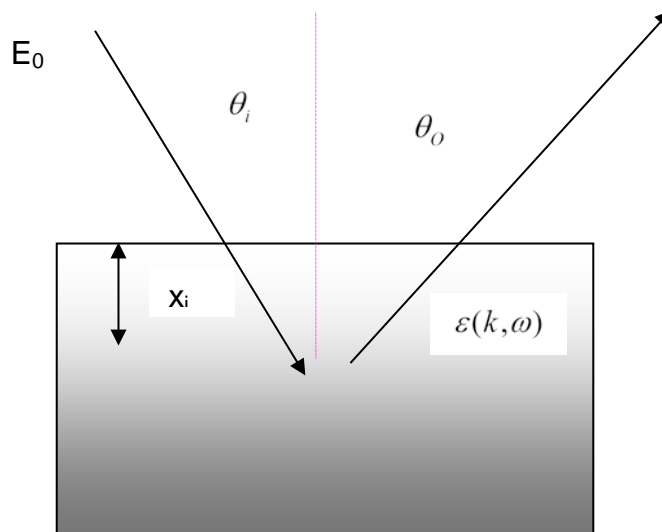


Fig.(1) Geometry of a REELS experiment

1.1 The QUEELS- $\epsilon(k, \omega)$ -REELS software package

The present software provides a tool for determination of the complex dielectric

function and optical properties, by analysis of the energy distribution of a mono-energetic beam of electrons being reflected from a solid surface as in REELS (reflection electron energy loss spectroscopy). From a REELS experiment it is possible to determine an effective experimental REELS cross section for inelastic scattering [3,4]. The basic idea behind the present software is to use theory [5,6] to simulate the REELS cross section based on a model dielectric function $\epsilon(k,\omega)$. By the constraint that this must fit with the experimental REELS cross section, $\epsilon(k,\omega)$ can thus be determined.

The REELS type of experiment is quite easy to make from an experimental and practical point of view, because the sample can be grown, prepared, cleaned and handled with ease. The method is valid even for energies of ~ 200 eV, for which the IMFP is < 1 nm. Therefore it can be applied even for films of ~ 2 nm thickness. The properties of a few nano-meter thick film can also easily be studied because they can be formed on supporting substrates. In contrast to this, the transmission electron energy loss (TEELS) experiment which has also in the past been applied to get similar information is much more complicated because it relies on analysis of the energy distribution of mono-energetic electrons that have passed through a thin film of the material. TEELS therefore require clean, thin and self-supporting films with uniform thickness. Such films are virtually impossible to make in practice when the film thickness is in the nano-meter range.

The situation in a REELS experiment is shown in fig.1 where the incoming electron is backscattered at a depth which is statistically distributed according to a Poisson distribution.

On the way out, the electron may interact with the field set up by the electron on the way in because this field is not necessarily completely relaxed by the time the electron goes back. This effect was recently studied in detail [N. Pauly, S. Tougaard, F. Yubero. Phys. Rev. B 73 (2006) 035402] where this effect was found to be significant for backscattering angles in the range $\sim 160 - 200$ degrees where there is a spatial proximity between the trajectories of the outgoing and the incoming electron.

1.2 Prospects for practical applications

With the analysis provided by the QUEELS- $\epsilon(k,\omega)$ -REELS software package it becomes easy to determine the dielectric function of thin films. We expect that this will improve the quantitative analysis of electronic properties of thin films. Thus the oscillators determined can be quantitatively compared on an absolute scale for different sample compositions. Samples can easily be grown and handled in the form of thin films on a suitable substrate. The only condition is that the film thickness is larger than ~ 2 IMFP (IMFP = inelastic mean free path). For an electron energy of around 1 keV the IMFP is ~ 1 nm and the minimum film thickness is thus only ~ 2 nm.

From the dielectric function optical properties like the refractive index and the

extinction and absorption coefficient can be determined. This is important because the present type of analysis is easily done in the far ultraviolet region where the applicability of optical methods is limited.

It is also possible to calculate a wide range of interactions of static and moving charged particles in the solid within the limits of the dielectric response description. This includes calculations of surface excitation effects, the interference effects between different fields set up in the solid by different particles as e.g. other moving charged particles and static charges (as met in photoelectron spectroscopy and Auger electron spectroscopy). Calculation of the important effective inelastic mean free path is also straight forward from the dielectric function [38].

2. Theoretical background.

Several research groups have been involved in the development of models to describe these processes. Thus, in 1954 Lindhard [39], described the energy losses of electrons moving in an infinite medium. A few years later, Ritchie [40] used a hydro-dynamical model to describe losses of electrons travelling through a thin film corresponding to the situation in transmission electron energy loss spectroscopy (TEELS). In the seventies and early eighties Flores, Echenique et al [41,42] were very active in the development of models for electron energy losses in different geometries. On the other hand Arista and co-workers [43] used the specular reflection model to interpret electron losses. Several other authors have also contributed with models [45, 46,47,48,49,50,51,53,54].

We have in the nineties, developed models based on a semi-classical dielectric response description of the interaction between the moving electron and the electrons in the solid as well as a possible core hole in solids (in photoemission) [5,6,7]. In these papers, we have presented models to calculate spectra as obtained in Reflection Electron Energy Loss Spectroscopy (REELS) and X-ray photoelectron spectroscopy (XPS) using a dielectric description of the interaction between the moving electron and the electrons in the surface region where it travels. The equations are complicated and involve several infinite integrations and this has been a main hindrance for widespread practical use of the results. We therefore decided to make an effort to implement the resulting algorithms into a user friendly software package that will facilitate the practical use of these models. We started this work in 2001 and the present software package is the first in a series (see www.quases.com) that each address different elements of the theory [55]. We hope that this software will help the research community to more effectively and quickly reach a better level of understanding of the importance of these processes for quantitative analysis of electron spectra. We also hope that the software will find use to motivate and enhance quantitative analysis of both optical and electronic properties of solids in general and of nano-meter thin films in particular.

The present manual and software package provides software that allows to determine the dielectric and optical properties of a solid by analysis of reflected electron energy loss spectra taken at one or more energies in the 100-2000 eV energy range. The validity of the procedure has been tested experimentally by extensive systematic experiments through variations of both the experimental geometries and electron energies over wide ranges and it has been shown to give quite consistent results [19]. This gives high confidence in the ability of the procedure to account for an accurate and quantitative description of the dielectric and electronic properties of thin films. As mentioned above, the validity was tested extensively in the energy range 100- 2000 eV. It is expected to be valid also at much higher energies, while the validity for energies below 100 eV has so far not been tested to any great extent.

3. Brief description of the theoretical model

The theory builds on a model where a response, in time and space, of the electrons in the solid to the moving electron is described by the complex dielectric function $\varepsilon(k, \omega)$ of the solid. The model was proposed in 1992 [5] for normal incidence and emission angles and in 1996 [6] it was extended to include general incidence and emission angles. It takes interference effects between surface and bulk excitations into account as well as excitations that take place when the electron moves in the vacuum before it enters and after it has left the surface of the sample.

For a given geometry, the program calculates the effective inelastic scattering cross section for electrons that have followed trajectories and is backscattered at different depths [6]. From this set of calculated effective cross sections, the average is calculated by a weighted average over the depths.

The dielectric function is described by an expansion proposed by Ritchie et al [53]

$$\text{Im} \left\{ -\frac{1}{\varepsilon(k, \omega)} \right\} = \text{GAP}(\hbar\omega) \times \sum_i \frac{A_i \gamma_i \hbar\omega}{\left\{ \left(\hbar\omega_{0i} + \alpha_i \frac{\hbar^2 k^2}{2m} \right)^2 - \hbar^2 \omega^2 \right\}^2 + (\hbar\gamma_i \hbar\omega)^2}.$$

where $\hbar\omega_i$, $\hbar\gamma_i$, and α_i are parameters that describe the energy, damping and dispersion of the individual oscillators that are used to describe the response in time and space of the electrons of the solid. The $\text{GAP}(\hbar\omega)$ function is included to describe the effect of a band gap in semiconductors and insulators. From the analysis of a wide range of experimental data [9-24] it has been found that for metals one expects that the dispersion $\alpha_i \sim 1$ for oscillators with $\hbar\omega_i < 20\text{-}30$ eV while $\alpha_i \sim 0$ for oscillators with $\hbar\omega_i > 30\text{-}60$ eV. For insulators and

semiconductors it is expected that $\alpha_i \sim 0$ for all oscillators when the bandgap is large ($> 3-9$ eV) while $\alpha_i \sim 0.2-0.6$ for all oscillators when the band gap is smaller ($< 1-3$ eV). These empirical values are recommended as starting values in the analysis procedure and the accurate α_i values as well as the $\hbar\omega_i$ and γ_i values are determined during the analysis. (see also the example in Sec. 9.1).

The software also includes a facility to ensure that the dielectric function fulfils the the Kramers-Krönig sum rule [44] which for insulators and semiconductors is

$$\frac{2}{\pi} \int_0^{\infty} \text{Im} \left\{ -\frac{1}{\varepsilon(k, \omega)} \right\} \frac{d\omega}{\omega} = 1 - \frac{1}{n^2}$$

where n is the refractive index of the material in the optical limit $\hbar\omega \rightarrow 0$. While for metals the Kramers-Krönig sum rule is

$$\frac{2}{\pi} \int_0^{\infty} \text{Im} \left\{ -\frac{1}{\varepsilon(k, \omega)} \right\} \frac{d\omega}{\omega} = 1$$

This is discussed further in a following section.

Fig.1 shows the geometry of a REELS experiment which is modelled by the QUEELS- $\varepsilon(k, \omega)$ -REELS software. We consider an electron moving with energy E_0 towards the surface of a solid characterized by a dielectric function ε . The probability that this electron shall lose energy $\hbar\omega$ ($\hbar\omega \ll E_0$) per unit energy loss and per unit path length is the so-called effective inelastic cross section $K_{\text{eff}}^{\text{bc}}(E_0, \hbar\omega; \varepsilon, x_i^{\text{bc}})$. The trajectory of the moving electron and the surroundings of the electron-surface system define the boundary conditions (bc) of the problem. Thus, x_i^{bc} refers to the particular set of parameters that describe the interaction between the moving electron and the surface. For example, for an electron moving in a V-type backscattering geometry (which is the case for most electrons of interest here [52], x_i^{bc} then refers to the incoming and outgoing angles and the depth at which the backscattering takes place. $K_{\text{eff}}^{\text{bc}}(E_0, \hbar\omega; \varepsilon, x_i^{\text{bc}})$ can be described in terms of the induced potential $\Phi_{\text{ind}}^{\text{bc}}(\mathbf{k}, \omega; \varepsilon, x_i^{\text{bc}})$ set up by the moving electron in a particular trajectory within the surface region of a solid, with initial energy E_0 and velocity \vec{v} . Thus, it is found that [5]

$$K_{\text{eff}}^{\text{bc}}(E_0, \hbar\omega; \varepsilon, x_i^{\text{bc}}) = \frac{2}{(2\pi)^4 x \hbar^2 \omega} \int_{-\infty}^{\infty} dt \int d^3 r \rho_e(\vec{r}, t) \text{Re} \left\{ \int d^3 k \vec{k} \cdot \vec{v} \Phi_{\text{ind}}^{\text{bc}}(\mathbf{k}, \omega; \varepsilon, x_i^{\text{bc}}) e^{i(\vec{k} \cdot \vec{r} - \omega t)} \right\} \quad (1)$$

where $\rho_e(\vec{r}, t)$ is the charge density that describes the moving electron, x is the

path length travelled inside the medium, and t , \mathbf{r} and \mathbf{k} are time, space and momentum variables of integration. The induced potential is found by solving the Poisson equation in Fourier space with the appropriate boundary conditions corresponding to the particular experimental situation.

The energy loss of an electron moving in an *infinite* medium is easily calculated within this model and results in the well-known expression

$$K_{\text{eff},\text{bulk}}(E_0, \hbar\omega; \varepsilon) = \frac{1}{\pi a_0 E_0} \int \frac{dk}{k} \text{Im}\{1/\varepsilon(\mathbf{k}, \omega)\}.$$

Simulating a REELS experiment is considerably more complex because the electron may lose energy while it moves in the vacuum above the surface and because of the influence of surface excitations. The expressions for a single trajectory are quite involved [5,6]. Furthermore, in a REELS experiment, the electrons have experienced not only a single trajectory, but a distribution of trajectories because the backscattering event can take place at different depths in the sample. This can be taken into account for a homogeneous sample, by a weighted average of the previously described effective cross section as

$$K_{sc}^{bc} = \left[\int_0^\infty dx Q^{bc}(x) K_{\text{eff}}^{bc} \right] / \left[\int_0^\infty dx Q^{bc}(x) \right] \quad \text{where } x \text{ is the total pathlength}$$

travelled by the electron inside the medium and $Q^{bc}(x)$ is the pathlength distribution function for the considered electrons. In the present software we have used $Q^{bc}(x) = x e^{-x/\lambda_{\text{eff}}}$, where λ_{eff} the so-called ‘‘effective’’ inelastic mean free path. In the program it can be either taken as a fixed value given by the available electron inelastic mean free paths from the literature or the software can calculate a self-consistent value determined as the inverse of the area of the effective cross section calculated by the software. It is in general recommended to use the self-consistent values in the calculations.

The $K_{sc}^{bc}(E_0, \hbar\omega)$ can be directly compared on an absolute scale to the $K_{sc}^{\text{REELS}}(E_0, \hbar\omega)$ which is obtained from analysis of an experimental REELS spectrum [4] by the formula in Ref. [3].

4. Examples of applications

QUEELS- $\varepsilon(\mathbf{k}, \omega)$ -REELS can obviously be used to determine the electronic, dielectric and optical properties of solids as well as of nano-structured thin films. It is also useful for fundamental studies of energy loss processes of electrons moving nearby surfaces and nano-structured materials. It may also be used to calculate the influence of surface excitations for the effective inelastic

mean free path in a REELS geometry and calculations of effective inelastic mean free paths, can also be applied to determine dielectric properties of bulk materials as well as of thin films. The essence of this method is to vary the parameters describing a parameterized dielectric function until good agreement is found between experimentally determined and theoretically calculated cross sections. So for each material there will be a unique set of parameters accounting for the dielectric properties. This procedure has been applied to determine the dielectric function and inelastic mean free paths and optical properties of many materials including metals, oxides, nitrides and semiconductors in the form of thin films [9-25]. It has also been applied for theoretical calculations of the importance of surface excitations [32,37].

Finally, it should also be noted that besides these wide applications, the accuracy of the applied theory behind QUEELS- $\epsilon(k,\omega)$ -REELS has been tested quantitatively in several experimental REELS [5,8, 9,10, 13,14,15] under wide variations of both the experimental geometry and the electron energy.

A corresponding software QUEELS-XPS (which can be downloaded at www.quases.com) makes similar dielectric response calculations of extrinsic and intrinsic excitation effects, including both the core hole and the effect of the surface) in photoemission. This has been applied in several papers [7,11,12,55-60].

5. Optical properties determined by Kramers-Krönig transformation

Optical properties from the ELF oscillators

The Energy Loss Function (ELF) in the optical limit (i.e. zero momentum transfer) is expressed as an expansion in Drude-Lindhard type oscillators which for $k=0$ is

$$\text{Im}\left\{\frac{1}{\epsilon(\hbar\omega)}\right\} = \theta(\hbar\omega - Eg) \times f(\hbar\omega) \times \sum_{j=1}^n \frac{A_j \gamma_j \hbar\omega}{(\hbar\omega_{0j}^2 - \hbar\omega^2)^2 + \gamma_j^2 \hbar\omega^2}$$

Here $\text{Im}\{1/\epsilon\}$ is the imaginary part of the reciprocal of the complex dielectric function. A_j (eV^2), γ_j (eV), and $\hbar\omega_j$ (eV) are the oscillator strength, width, and energy position of the j -th oscillator. Besides, $\hbar\omega$ is the energy (in eV) at which $\text{Im}\{1/\epsilon\}$ is evaluated.

The function $\theta(\hbar\omega - E_g) \cdot f(\hbar\omega)$ is included to describe the effect of an energy band gap E_g (eV) in semiconductors and insulators. The step function $\theta(\hbar\omega - E_g) = 0$ for $\hbar\omega < E_g$ and $\theta(\hbar\omega - E_g) = 1$ for $\hbar\omega > E_g$. The function $f(\hbar\omega)$ is introduced to get smooth transition, in the $E_g < \hbar\omega < E_g + a1$ energy range, between the intensities of the onset absorption and the pure Drude-Lindhard oscillators.

$$f(\hbar\omega) = \left[a2 \frac{(\hbar\omega - E_g)^p}{(\hbar\omega)^2} \right]^{tmp1} \quad \text{if } E_g < \hbar\omega < E_g + a1$$

$$\text{where } tmp1 = \cos^2 \left[\frac{\pi}{2} \frac{\hbar\omega - E_g}{a1} \right]$$

$$f(\hbar\omega) = 1 \quad \text{if } \hbar\omega > E_g + a1$$

$p = 0.5$ (2.0) for direct (indirect) gap materials respectively, $a1$ is the transition energy range and $a2$ is related to the strength of the absorption at the gap edge. The chosen $f(\hbar\omega)$ function warrants the right energy dependence nearby the absorption onset in the case of either direct or indirect band gap semiconductors respectively. (The parameters $a1$ and $a2$ are called d_Gap and A_Gap respectively on the input-screen when the *Set Oscillators* menu is selected in the software).

This parameterization allows to perform an easy Kramers-Krönig transformation to obtain the real part $Re\{1/\varepsilon\}$ of the reciprocal of the complex dielectric function.

From $Im\{1/\varepsilon\}$ and $Re\{1/\varepsilon\}$, the real ε_1 and imaginary ε_2 parts of the dielectric function ($\varepsilon = \varepsilon_1 - i\varepsilon_2$) are given by

$$\varepsilon_1 = \frac{Re\{1/\varepsilon\}}{(Re\{1/\varepsilon\})^2 + (Im\{1/\varepsilon\})^2}$$

$$\varepsilon_2 = \frac{Im\{1/\varepsilon\}}{(Re\{1/\varepsilon\})^2 + (Im\{1/\varepsilon\})^2}$$

The complex refractive index N ($N=n-ik$, with n the refractive index and k the extinction coefficient) is related to ε as

$$N = \sqrt{\varepsilon}$$

$$n = \sqrt{\frac{1}{2} \left(\sqrt{\varepsilon_1^2 + \varepsilon_2^2} + \varepsilon_1 \right)}$$

$$k = \sqrt{\frac{1}{2} \left(\sqrt{\varepsilon_1^2 + \varepsilon_2^2} - \varepsilon_1 \right)}$$

The absorption coefficient μ (given in units μm^{-1}) is related to the extinction

coefficient k as

$$\mu = 10.1 \cdot \hbar\omega \cdot k$$

where $\hbar\omega$ is in eV.

These optical quantities can be calculated from the dielectric function using the menu *Calculate Optical Properties* in the QUEELS- $\epsilon(k,\omega)$ -REELS software package.

When this is applied to a given set of oscillators, it is important to make sure that the dielectric function satisfies the Kramers-Krönig sum rule. This can easily be done by using the facility in the *Set Oscillators* menu by clicking the button *Auto-Rescale Intensities A0 to fulfill the KK-sum rule*. This rescales the oscillator strengths to fulfill the KK sum rule (see also Sec.3).

6. Practical brief overview

Analysis of a set of REELS spectra consists in the following steps:

1. REELS spectra are measured at a single or preferably at two or more primary energies / and or geometries
2. The multiple scattered electrons are removed from the measured REELS spectra with the software QUASES-XS-REELS_1 to produce a set of LK curves that correspond to effective single scattering cross sections. *Alternatively you may use the full QUASES-XS-REELS software package in this step.* This has more built in facilities to analyze REELS spectra if they are not recorded under ideal experimental conditions.
3. Guided by the structure in the LK curve which was derived from the REELS recorded at the highest primary energy, a rough guess of the oscillators in the dielectric function is estimated. This is done with the first menu in the QUEELS- $\epsilon(k,\omega)$ -REELS software called: *Set Oscillators*.
4. The software calculates energy loss spectra for mono-energetic electrons backscattered at 65 depths. The depths are automatically selected by the program. This is done with the second menu in the QUEELS- $\epsilon(k,\omega)$ -REELS software package called: *Calculate Set of Cross Sections*. This is done with a coarse energy grid e.g. 0.5 eV over the full energy range where structure in the experimental LK from step 2 is observed.
5. From the file created in step 4, a REELS cross section that can be compared with

LK determined in step 2 is calculated. This is done with the third menu in the QUEELS- $\epsilon(k,\omega)$ -REELS software package called: *Calculate K-REELS*. If REELS were taken at several primary energies, steps 4 and 5 should be done for the REELS taken at the lowest and the highest energy because these two show the largest variation in effective cross sections.

6. The calculated cross section is compared to the experiment by using the fourth menu in the QUEELS- $\epsilon(k,\omega)$ -REELS software package called: *CalculateIMFP*K and Compare to Experiment*. After examination of the differences between theory and experiment, it is decided approximately what changes should be made to the trial dielectric function to improve the agreement.
7. Repeat the cycle described in steps 3-6 a few times. Guided by the observed deviations between theory and experiment, the parameters for the oscillators are, in each cycle, adjusted and more oscillators are added if required.
8. If REELS were taken at several primary electron energies, the calculations in step 4-5 are then done for the full set of REELS spectra available at other energies and/or geometries and final small adjustments to the oscillators are made. If it is judged necessary, the calculations are also made with a finer energy step in this final step.
9. Make final small adjustments of the oscillators if required.
10. From the determined dielectric function, optical properties may be calculated by using the fifth menu in the QUEELS- $\epsilon(k,\omega)$ -REELS software package called: *Calculate Optical Properties*.

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.

7. Installation of QUASES_XS_REELS_1

This program implements the theory by Tougaard and Chorkendorff [3] to calculate the effective cross section from a measured REELS.

Click the *Setup.exe* program and follow the instructions on the screen to install the program.

7.1 Run the program

(see also Section 9.1.1 below).

Start the program by clicking the QUASES-XS-REELS_1 icon in the QUEELS- $\epsilon(k,\omega)$ -REELS program menu and get the following. *Alternatively you may use the full QUASES-XS-REELS software package in this step.*

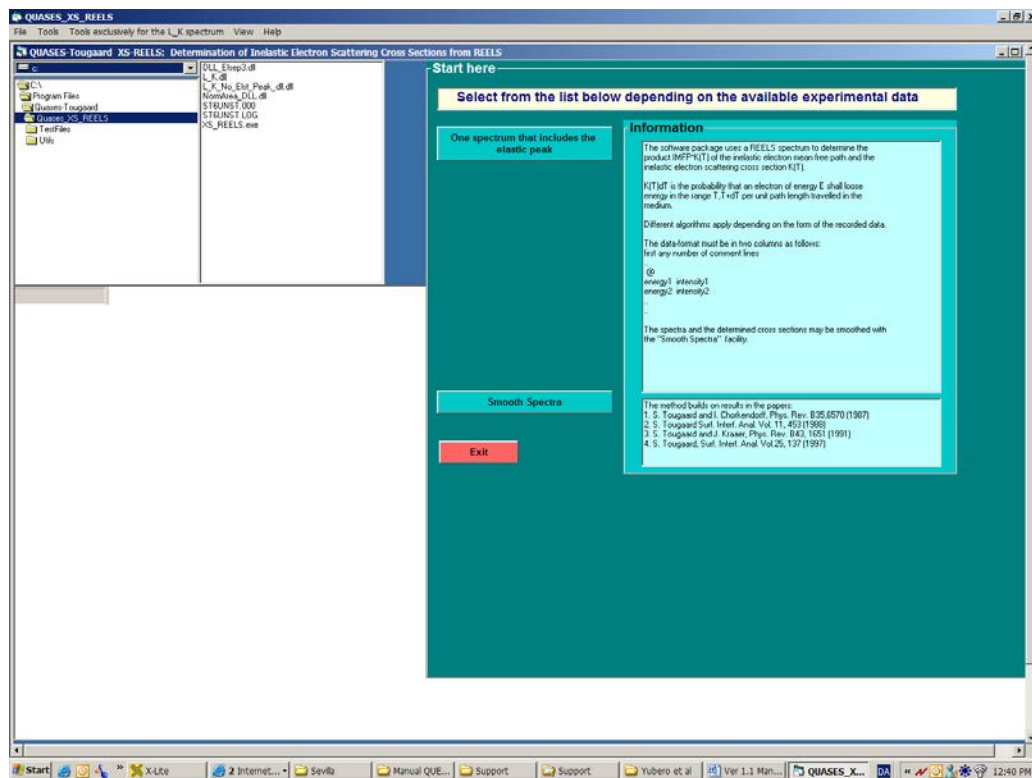


Fig.(2)

Click *One Spectrum that Includes the Elastic Peak*.

Find the REELS spectra in the file manager in the upper left part of the screen.

Click the file with the REELS spectrum (e.g. *ZRO2_1600.txt*) in the filelist, then click *Read Spectrum* and get

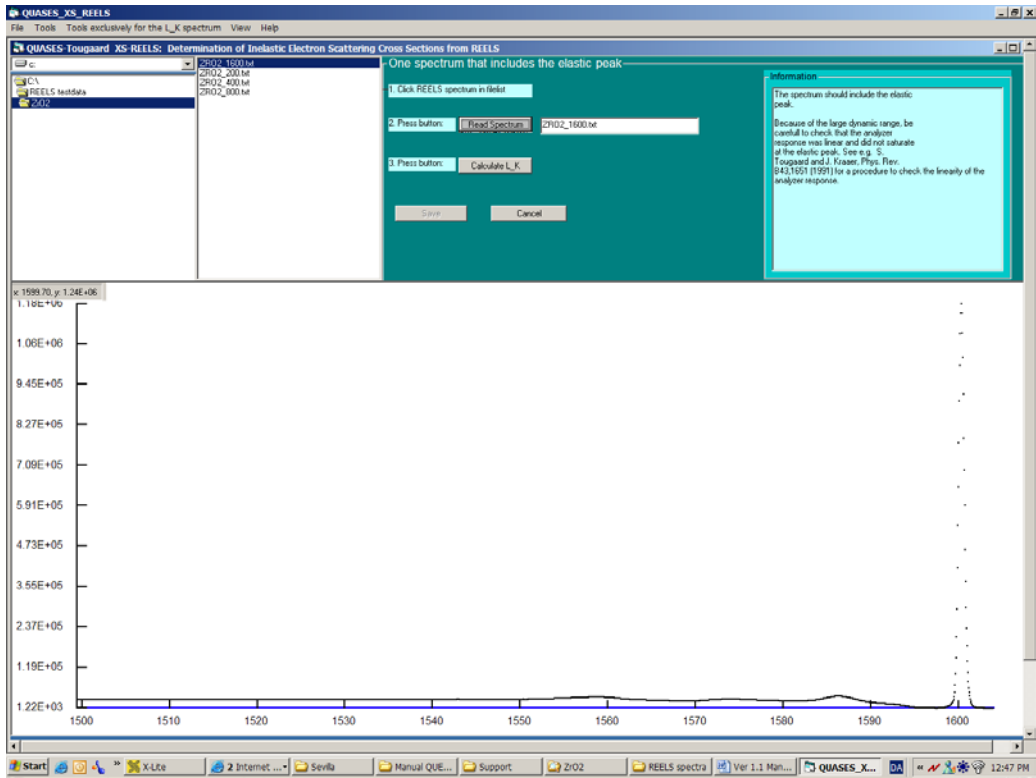


Fig.(3)

Click *Calculate LK* and get

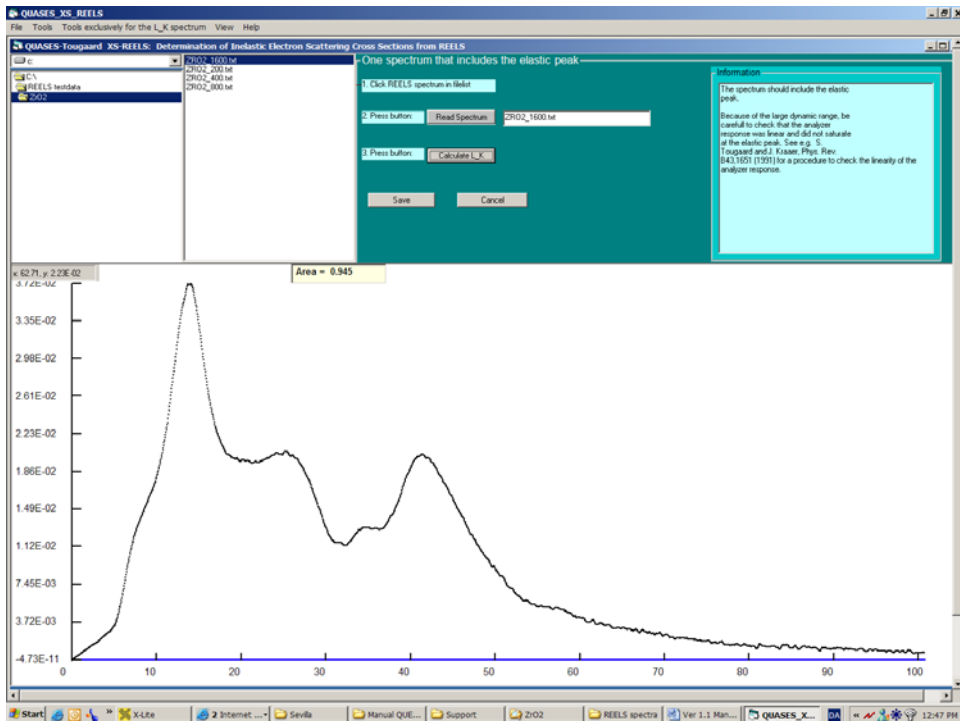


Fig.(4)

(In rare cases it has been observed that if you analyse a spectrum with poor energy resolution, you may experience that the extension of the linear part in LK, for low energy loss, is unrealistically large (which is not the case here). This is caused by the poor energy resolution and as a result the program has problems to automatically separate the elastic and inelastic parts of the spectrum. If this is the case, you can fix the problem by opening the experimental file and change the intensity at a single energy point about 0.5 or 1 eV on the low energy side of the elastic peak to zero. This will help the program to separate the elastic and inelastic regions of the spectrum). You may also use the program QUASES-XS-REELS which provides more facilities than QUASES-XS-REELS-1 for determining the experimental cross section from the REELS spectrum (see www.quases.com).

Click *Save* and enter a filename, for example *L_K ZrO2-1600*. This is the effective scattering cross section which we will later compare on an absolute scale to the calculations of the QUEELS- $\epsilon(k,\omega)$ -REELS part of the program (see next chapter). Repeat this for the other experimental REELS spectra

After creating each L-K file, note the value of “Area= .. “ shown in the text box above the plot. This Area is normally between 0.75 and 1.1. If it lies outside this range, your experimental data are likely to be in error. The most likely reason is that your analyser saturates in the region of the elastic peak. Test for this e.g. by the procedure described in [4].

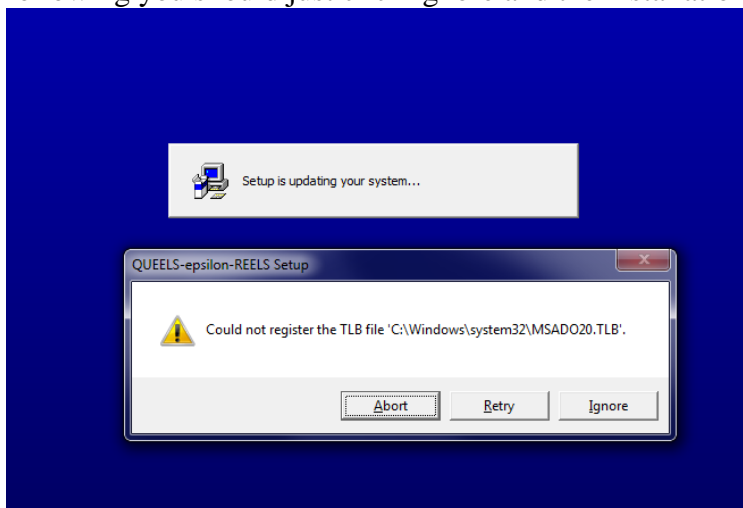
After finishing, click *Cancel* and then click *Exit*

The spectra thus created will in the following alternating be denoted either “experimental LK” spectra or “experimental IMFP*K(T)” spectra.

8. Install QUEELS- $\epsilon(k,\omega)$ -REELS

This program implements the theory by Yubero, Tougaard and co-workers [5,6] to calculate the effective cross section in REELS. It contains facilities to calculate the theoretical spectra that can be compared with the experimental LK spectra created in section 7.1 above.

To install, click the *Setup.exe* program and follow the instructions on the screen. (Press Enter to all questions asked). If at the end of the installation you get the following you should just click Ignore and the installation will complete.



8.1 Running QUEELS- $\epsilon(k, \omega)$ -REELS

Start the program by clicking the QUEELS- $\epsilon(k, \omega)$ -REELS icon in the QUEELS program menu and get the following:

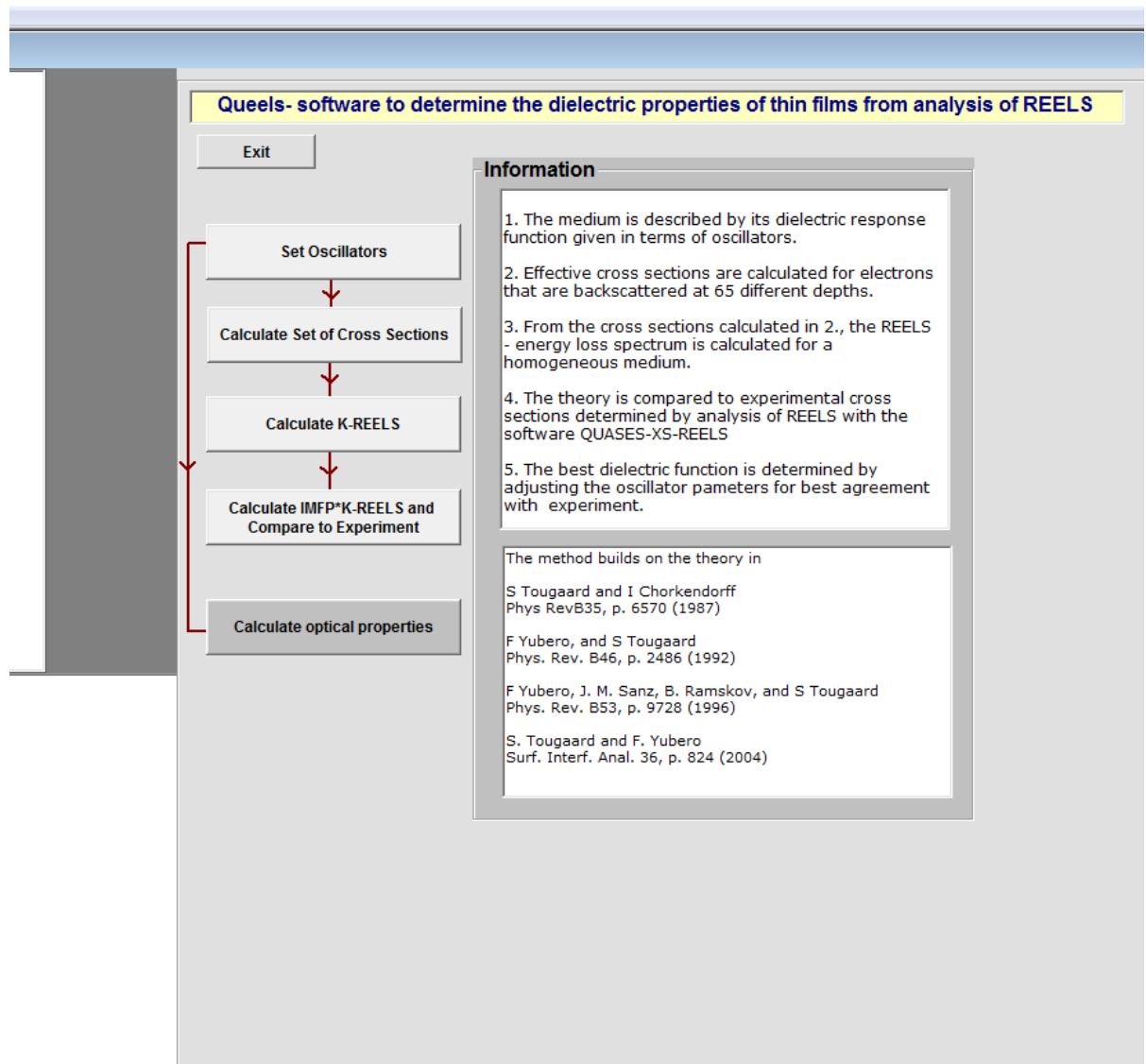


Fig.(5)

The functionality of the software will be described in the next chapter.

9. Features and practical application of the software package. Quantitative analysis of a set of REELS spectra to determine the dielectric and optical properties of the film.

There are strong surface effects on the cross section experienced by an electron that travels in the surface region of a solid. The magnitude depends on the electron energy as well as the geometry of the trajectory. From the theory handled by the QUEELS- $\epsilon(k,\omega)$ -REELS software, it is possible to calculate these variations quantitatively and the only input in the calculations is the dielectric function. By varying the dielectric function until good agreement with experimental REELS is found at one or more energies and/or experimental geometries, it is therefore possible to determine the dielectric function $\epsilon(k,\omega)$.

In this chapter we describe the features of the software package. This is done by taking a practical example and we shall go through the analysis procedure step by step. The experimental raw REELS data are provided with the software so you can get familiar with the use of the software by following the steps in the analysis on your own.

9.1 Tutorial Example. Analysis of REELS from ZrO₂.

In this example we will go through the steps needed for analysis of REELS from ZrO₂. The data analysis was published in the paper [10]:

F. Yubero, J. M. Sanz, J. F. Trigo, E. Elizalde and S. Tougaard, Surf. Interf. Anal., 22, p. 124 (1994)

Spectra needed:

ZrO2_200.txt, ZrO2_400.txt; ZrO2_800.txt; ZrO2_1600.txt

These spectra are REELS spectra of electrons reflected from a ZrO₂ sample. The REELS spectra were taken at the energies 200 eV, 400 eV, 800 eV and 1600 eV in a geometry where incidence angle is $\theta_1 = 60^\circ$ with respect to the surface normal and the analyzer axis is normal to the surface i.e. $\theta_2 = 0^\circ$.

9.1.1 Determination of the experimental L-K (or IMFP*K(T)) cross sections

The first step is to remove the multiple scattered electrons from the REELS spectra to get the effective single scattering cross section. This is done by the algorithm in [3] which is implemented in the QUASES-XS-REELS_1 program. *Alternatively you may use the full QUASES-XS-REELS software package in this step.*

1. First create a folder (e.g. C:\REELS-data) and put your REELS spectra in

the folder. Start the QUASES-XS-REELS program. Find, with the help of the file-manager, the data files with the REELS spectra.

2. Click *One Spectrum that includes the elastic peak* (see Fig. 2)
3. Find the file with the REELS spectrum using the file manager in the upper left part of the screen.
4. Click the filename (ZrO2_1600.txt).
5. Click *Read Spectrum* and get Fig.(3)
6. Click *Calculate L_K* and get Fig.(4). This is the determined $IMFP \cdot K(T)$ function in absolute units [eV^{-1}].
7. To save the determined $IMFP \cdot K(T)$ function:
 - a. Click *Save* (A new dialog box will appear)
 - 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 (in this case we type the name *LK-ZrO2-1600*).
 - d. Click *Save Cross Section*.
 - e. The new file is saved and the filename appears in the file list box.
9. Repeat points 4-8 for the other REELS data files and determine the experimental cross sections *LK-ZrO2-200*; *LK-ZrO2-400*; *LK-ZrO2-800*.

9.1.2 Determine the first very rough estimate for the ELF oscillators

10. To determine the first estimate for the oscillators that make the ELF function, do the following:

Repeat first point 4-6 for the spectrum taken at the highest energy (in this case *ZrO2_1600.txt*) and get figure 4. The reason why we choose the L-K function at the highest available energy (here 1600 eV) to make the initial estimate for the oscillators, is that at the highest energy the effect of the surface are the smallest and the effect of the k-dispersion is also smallest. Therefore, the ELF has a shape which is to some extent similar to the high energy experimental LK.

Note that it is not necessary to include REELS taken at different primary electron energies. But the quality of the determined dielectric function is likely to be higher when this is the case (e.g. by using REELS taken at 300 eV and 1500 eV).

11. Locate, with the mouse, the position of the main peaks as well as their approximate full width at half maximum. (Note that as you move the mouse, the energy and intensity are shown in a small box in the upper left corner of the plot). A quick investigation in this way of Fig.(4) with the mouse cursor

identifies 5 main oscillators with maxima at 14, 25, 34, 42, 58 eV. The approximate half-width of the peaks is also determined with the mouse and the relative oscillator strength of the five peaks is also estimated. (These approximate relative oscillator strengths are simply found by eyeballing the figure and remembering that the wide peaks have larger strength than the narrow peaks although their peak intensity is smaller. Thus, although the intensity at 14 eV is the highest, the corresponding oscillator strength is not the largest because this peak is narrow). The exact value for this initial guess is not so important since it will be adjusted in the following steps. These approximate values are listed in table 1. We will use this rough estimate as starting values for the oscillators.

12. Click *Cancel* and then *Exit* to close the QUASES-XS-REELS program

Table 1

$\hbar\omega_i$ (eV)	A_i (relative strength of peaks)	γ_i (eV) (half width of peaks)	α_i
14	50	5	1
25	70	10	1
34	15	5	1
42	150	10	1
58	20	15	1

9.1.3 Calculation of theoretical cross sections and determination of the oscillators

Now, start the QUEELS- $\epsilon(k,\omega)$ -REELS program and get fig.5.

Click *Set Oscillators*. Then type in the values in table 1; type also the following values $E_{gap} = 4.5$ eV, and $n = 1.9$ (the energy gap and refractive index of ZrO_2). Select *dirBG* and set $d_Gap = 0$ and $A_Gap = 0$. (These parameters are used to smooth the transition around the band gap (see Sec. 3). With these selected values it is just a step function. In this example and will not explore the finer details at the band gap). Finally click the button *Auto-Rescale Intensities A0 to fulfill the KK-sum rule*. Click this button and observe that the *KK-sum* ~ 1.0 . Notice that the A_i values are also changed. You now have Fig. (6). Note that the ELF is similar to the L_K cross section at 1600 eV (shown in fig. 4).

Note that the ELF is given by the estimated data in table 1. These were determined from Fig.(4) which is for ZrO_2 with $E_p = 1600$ eV. The ELF is a

property of the material and is the same when we calculate LK for different energies and geometries because the energy and geometry dependence of the theoretical spectra is calculated by the software.

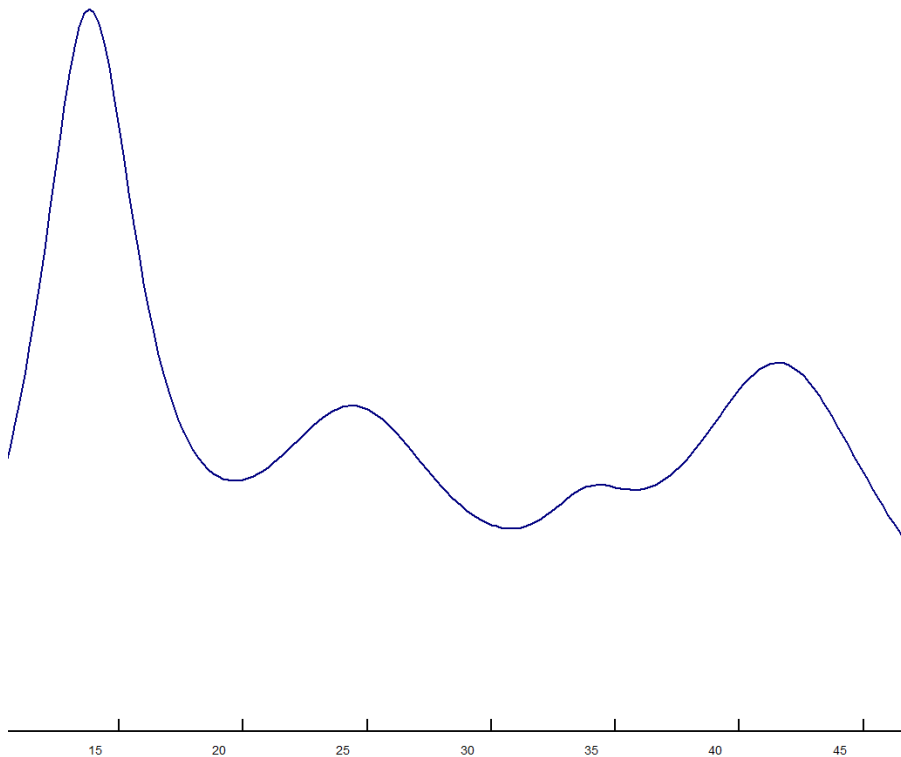
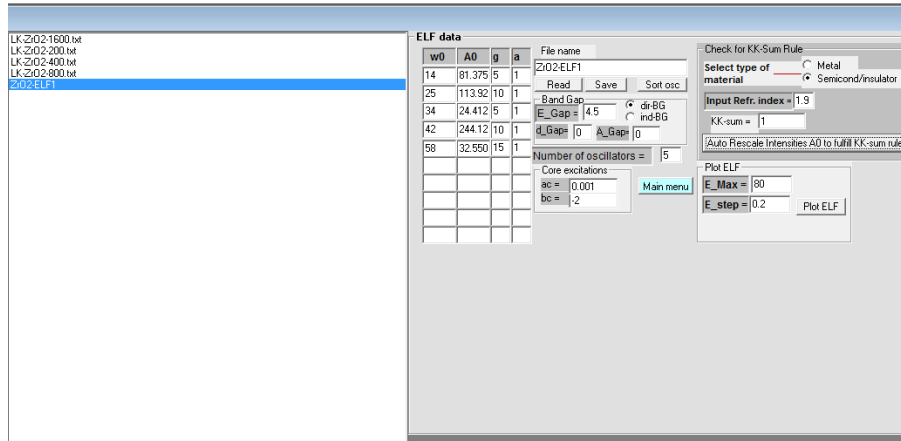


Fig.(6)

Type a filename (in this case: *ZrO2-ELF1*) and then click save. Notice that this file is added to the file-list.

Now click *Main Menu*

Click *Calculate Set of Cross Sections*. This part of the program calculates the energy spectra for electrons that are backscattered at 65 different depths. The depths are selected automatically by the program and are distributed over the relevant path-lengths. (The software calculates the IMFP corresponding to the ELF oscillators and based on this, it calculates a set of depths).

Click the file with the ELF data in file-list (here: *ZrO2_ELF1*).

Click *Read ELF file*.

Set the parameter values: $E_p = 1600$; $\theta_1 = 60^\circ$; $\theta_2 = 0^\circ$; $E_{max} = 70$ eV; $E_{step} = 0.5$ eV. We choose a coarse energy grid (0.5 eV) to make the initial calculations faster. Later, we may (if this is found necessary) make the calculations with a finer energy grid when we make the final adjustments of the ELF.

In the appropriate textbox you write the name of the file where you wish to save the calculated spectra for the 65 depths. (Here we choose the name: *Keff_65_ZrO2_1600_ELF1*). See Fig.(7)

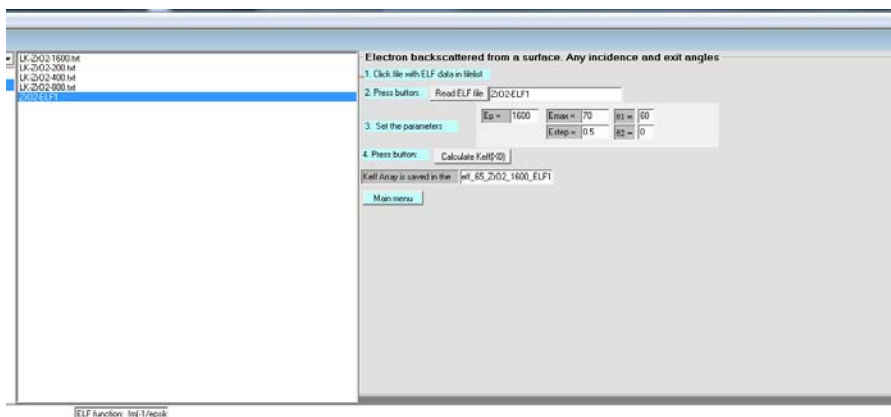


Fig. 7

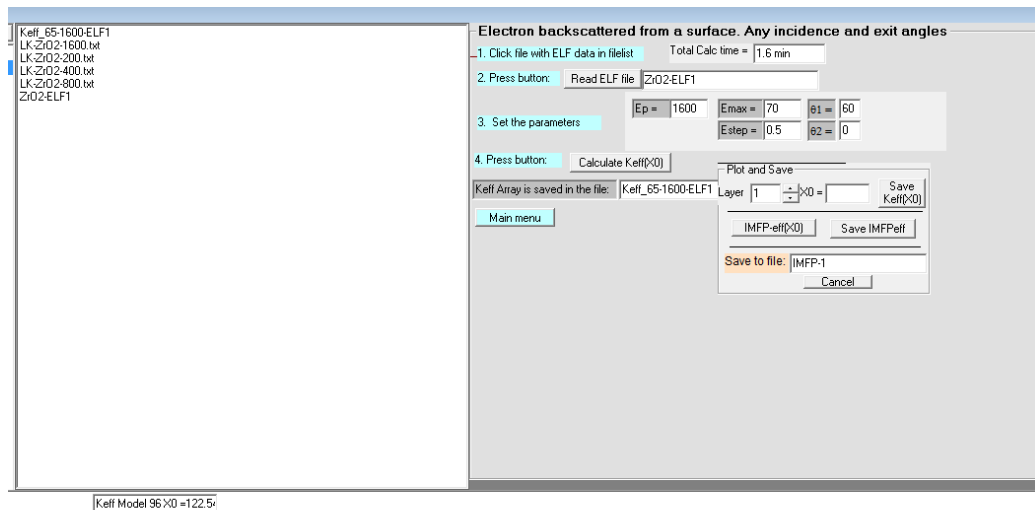


Fig. 8

Click *Calculate Keff(X0)* to calculate the K_{eff} for the 65 depths. Let the PC run until the program is finished (this takes ~ 2 -15 min. depending on the calculated energy range and the speed of your PC). *Note that the program may stop if you run another program simultaneously.*

When the calculations finish, the data are automatically saved to the file *Keff_65_ZrO2_1600_ELF1* which then appears in the file list.

A new save-dialog box appears (see fig.8). This is used to calculate the effective IMFP as a function of the depth and it provides also facilities to show graphs of the calculated cross sections for the various path lengths traveled. These options are included to make it possible to study individual effective cross sections for selected trajectories and it is quite instructive to go through the 65 files and see the gradual development in the shape as the influence of the surface gets increasingly smaller for larger path lengths. There is also a facility to save the cross sections in separate files for the individual paths.

The options in this dialog box are not needed at this moment, and you click *Cancel*

Now change the energy to $E_p = 200$ eV and change the filename to *Keff_65_ZrO2_200_ELF1*.

Then click *Calculate Keff(X0)* to calculate the K_{eff} for the 65 depths for the 200 eV electrons.

At first we only compare to spectra at 1600 eV and 200 eV because these will

show the largest change in spectral shape. After the initial determination of the ELF parameters has been done at these two extreme energies we may make small fine adjustments to make a good agreement also for the REELS spectra at the intermediate energies.

After the calculations at 200 eV have finished and the file *Keff_65_ZrO2_200_ELF1* appears in the file list, you click *Cancel* and then click *Main Menu*. Then click *Calculate K-REELS* to get to the program that, from the data files *Keff_65_ZrO2_200_ELF1* and *Keff_65_ZrO2_1600_ELF1*, will calculate the theoretical L_K cross sections that can be compared to the experimental L_K cross sections on an absolute scale. You should now have fig. 9.

Now click the filename *Keff_65_ZrO2_1600_ELF1* in the file list. Then click *Read Keff(X0)* to read the data-file and then click *Calculate Total effective REELS cross section*. Select the default options: *Use self consistent IMFP* and *Elastic scattering ignored*. Then Click *Save spectrum*. The program suggests the filename *Keff_65_ZrO2_1600_ELF1_Keff_av*. Click *Save Spectrum*. (See Fig.(10) .

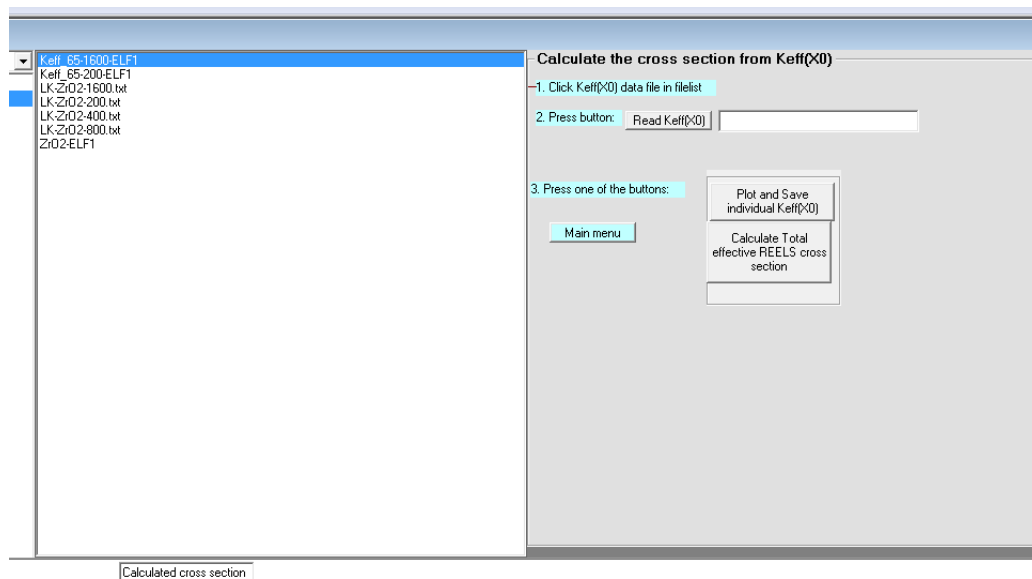


Fig.9

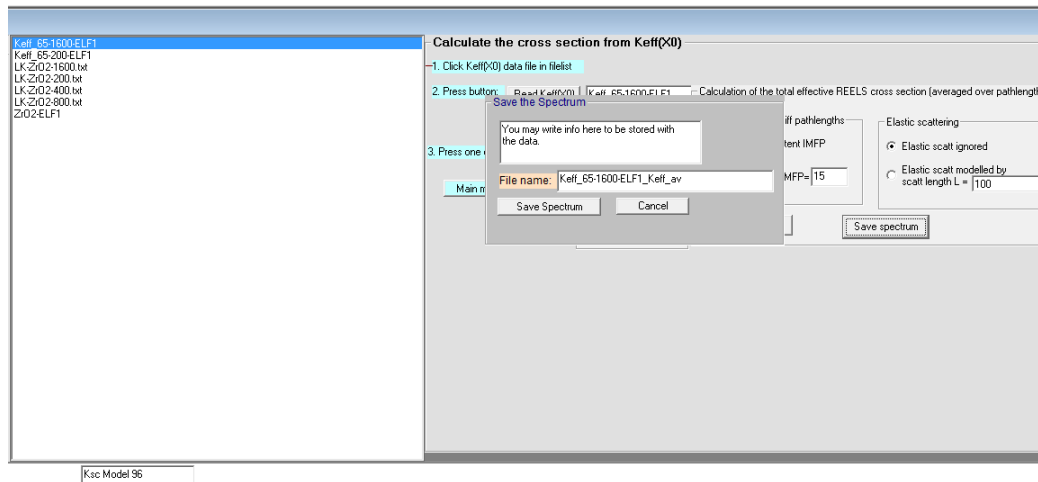


Fig. 10

Then click *Cancel* and click *Cancel* again to get back to the menu in fig.9.

Now repeat the calculation for the data at 200 eV: Click the filename *Keff_65_ZrO2_200_ELF1* in the file-list. Then click *Read Keff(X0)* to read the file and then click *Calculate Total effective REELS cross section*. Click *Save spectrum*. The program again suggests a filename in a new frame box. Then click *Save spectrum* and click *Cancel*, and click *Cancel* and then click *Main Menu*.

9.1.4 Comparison between theoretical and experimental cross sections

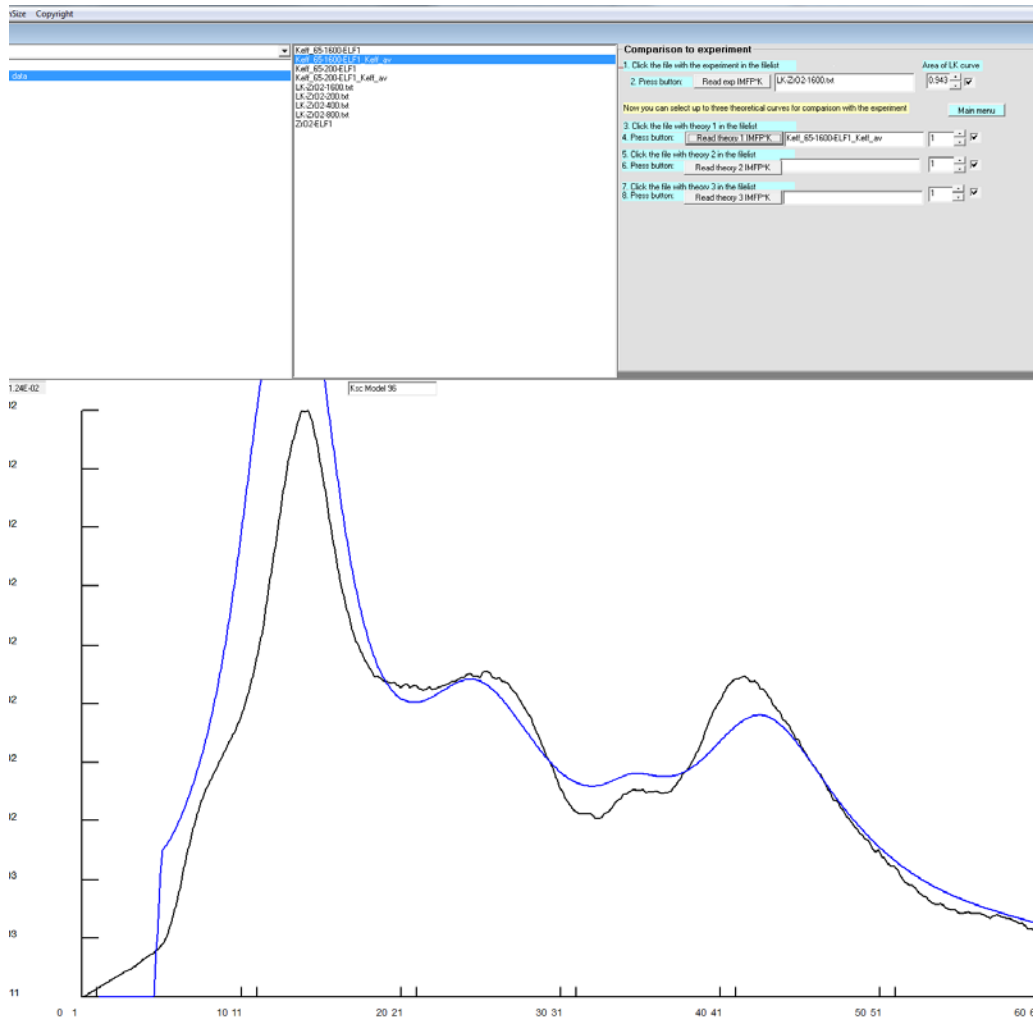


Fig.(11)

In the Main Menu click *Calculate IMFP*Keff-REELS and Compare to Experiment*.

Click the file with the experimental cross section at 1600 eV: *L_K ZrO2-1600*, then click *Read exp IMFP*K*.

Then click *Keff_65_ZrO2_1600_ELF1_Keff_av* in the filelist and then click *Read Theory1 IMFP*K* and get Fig. 11

Try to change the factor in the box to the right of the *Read theory 1 IMFP*K* button. Change it from 1 to 0.75 and you will see that the peak intensity matches better for the peak at ~14 eV. This facility can be used to quickly get a feeling for the changes that are needed in the relative intensities of the oscillators to make a better fit. Determine also with the mouse the position of the peaks. From a quick rough analysis we arrive in this way to the conclusion that the individual peaks

should be changed as in table 2.

Table2.

$\hbar\omega_i$ (eV)	Change in A_i	Change in $\hbar\omega_i$ (eV)	Change in $\hbar\gamma_i$ (eV)
14	-20 %		-1
25		+1	
34	-10 %		
42	+5 %		
58			

Now repeat the same procedure for the experiment and theory at 200 eV. The result is shown in fig.12

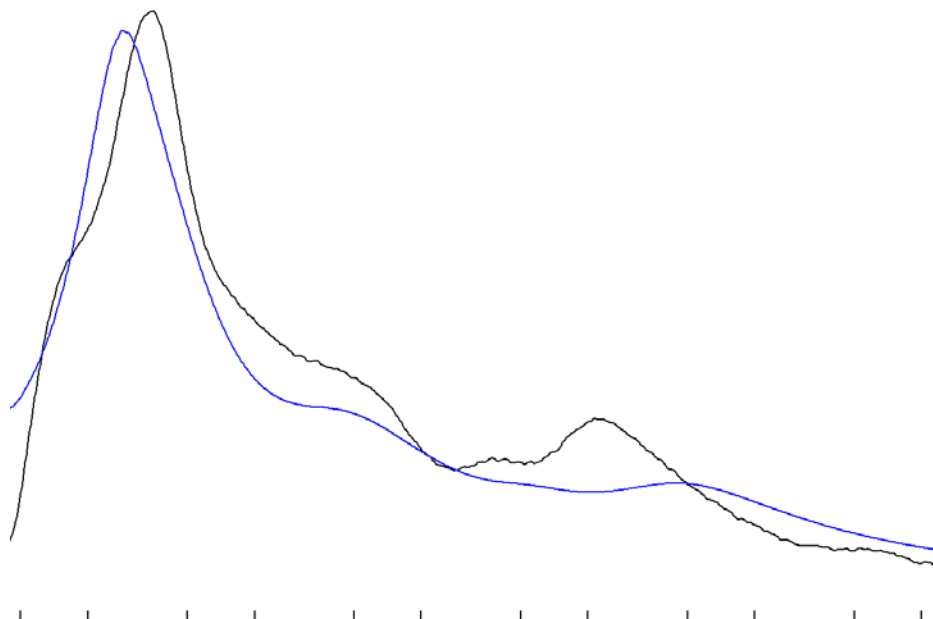
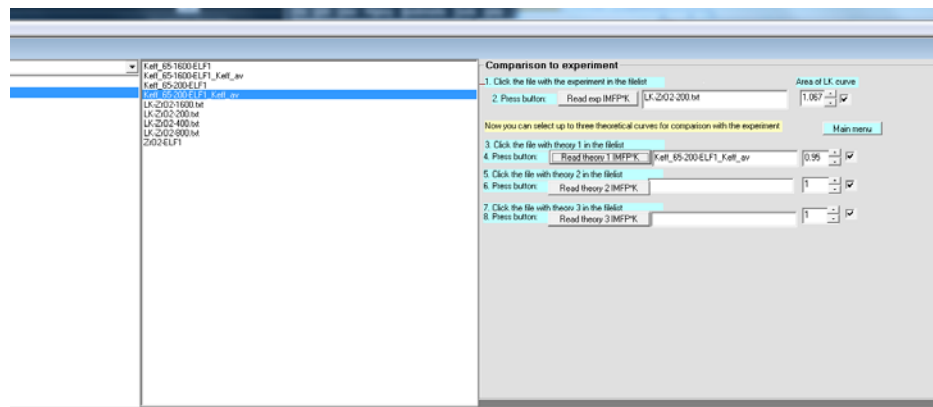


Fig.(12)

We notice that the peaks and in particular the peak at ~ 42 eV shift to higher energy for the cross section at 200 eV (Fig. 12) compared to the cross section at 1600 eV. This is not seen in the experiment. The reason for the shift is the k -dependence in the dielectric function. This will cause the peak to have an asymmetric tail towards higher energy loss and the effect is largest for small primary electron energies. The real solid does not show this behavior. From this we can conclude that the dispersion represented by the parameter α is much smaller than the assumed free electron value $\alpha = 1$.

Now we adjust the values in the oscillators by the amounts determined in table 2. To do this, click *Main Menu* and click *Set Oscillators*. Then click the file ZrO2-ELF1 in the filelist and click *Read*. Change the values of ω_i , A_i and γ_i by the amounts in table2.

To account for the much smaller dispersion, we set $\alpha = 0.1$ for all oscillators.

Click *Auto Rescale Intensities A0 to fulfill KK-sum rule* and observe that $KK_sum \sim 1$.

Change the file name to *ZrO2_ELF2* and click *Save*.

Click *Main Menu*.

Repeat the calculations with the new *ZrO2_ELF2*.

First create the files

Keff_65_ZrO2_1600_ELF2 and *Keff_65_ZrO2_200_ELF2* and then from these calculate *Keff_65_ZrO2_1600_ELF2_Keff_av* and *Keff_65_ZrO2_200_ELF2_Keff_av*. The latter two are shown in Figs 13 and 14 in comparison with the experimental cross sections *LK_ZrO2-1600* and *LK_ZrO2-200*.

The shift for the cross sections at 200 eV observed in Fig 12 of the 42 eV peak is much smaller in Fig. 14. However there is still a small shift to larger energy which is not seen in the experiment. This indicates that the dispersion represented by the α parameter should be further reduced. Therefore we set $\alpha = 0.05$ for all oscillators in the following.

From the analysis of a wide range of experimental data [9-24] it has been found that for metals one expects that the dispersion $\alpha_i \sim 1$ for oscillators with $\hbar\omega_i < 20$ -30 eV while $\alpha_i \sim 0$ for oscillators with $\hbar\omega_i > 30$ -60 eV. For insulators and semiconductors it is expected that $\alpha_i \sim 0$ for all oscillators when the bandgap is large (> 3 -9 eV) while $\alpha_i \sim 0.2$ -0.6 for all oscillators when the band gap is smaller (< 1 -3 eV). These empirical values are recommended as starting values in the analysis procedure and the accurate α_i values as well as the $\hbar\omega_i$ and γ_i values are determined during the analysis.

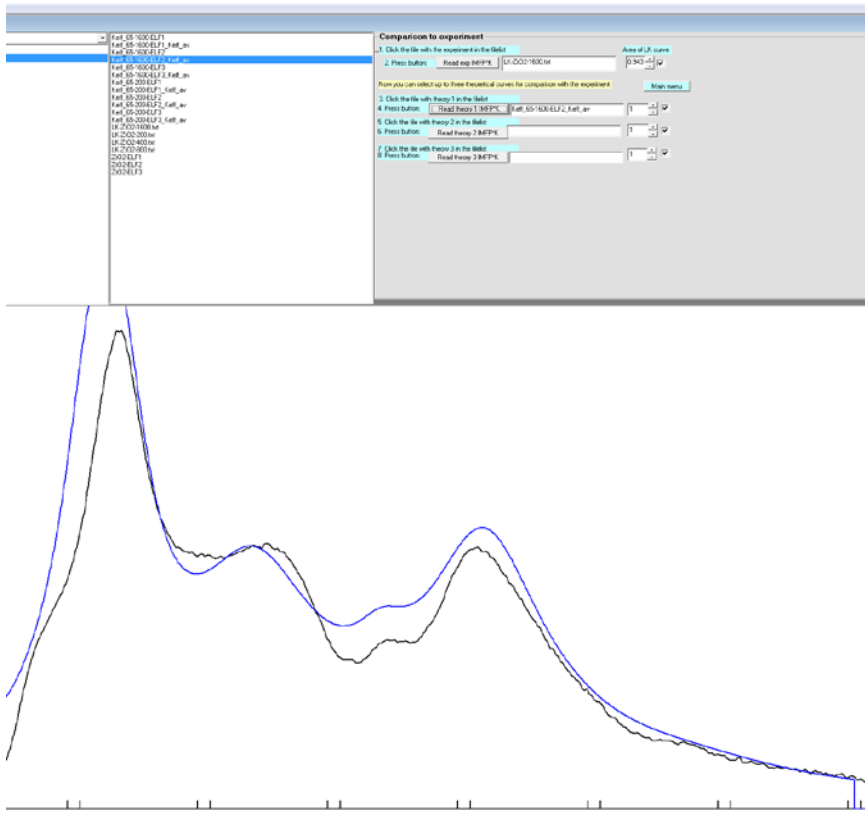


Fig. 13

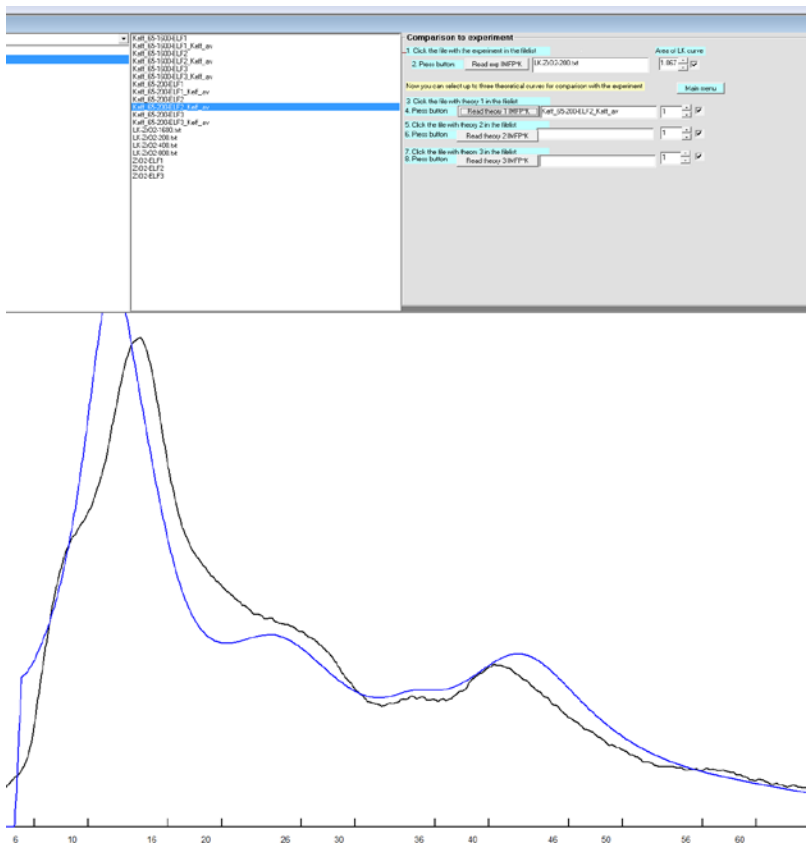


Fig. 14

Now we can keep this dispersion dependence and focus on improving the theoretical cross section at 1600 eV by changing the parameters for the oscillators.

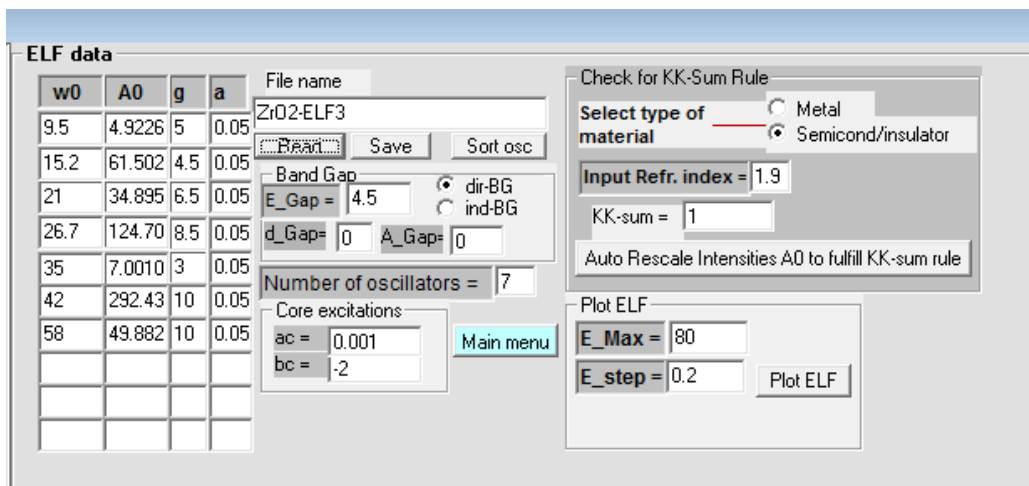
This procedure is now continued and the oscillator parameters are adjusted and a few more oscillators are added in regions where intensity is missing.

You add more oscillators in the empty rows below those already filled. By clicking *Sort osc*, the oscillators will be sorted in order of increasing oscillator energy.

After a few iterations the ELF oscillators in table 3 are found and the corresponding spectra are shown in figs 15 and 16 at 1600 eV and 200 eV respectively. The agreement between theoretical and experimental cross sections is now much better for both 1600 eV and 200 eV.

Table 3:

Egap= 4.5
and the following oscillators



The facilities provided by setting the two parameters d_Gap and A_Gap may also be used to get a better agreement close to the band gap energy.

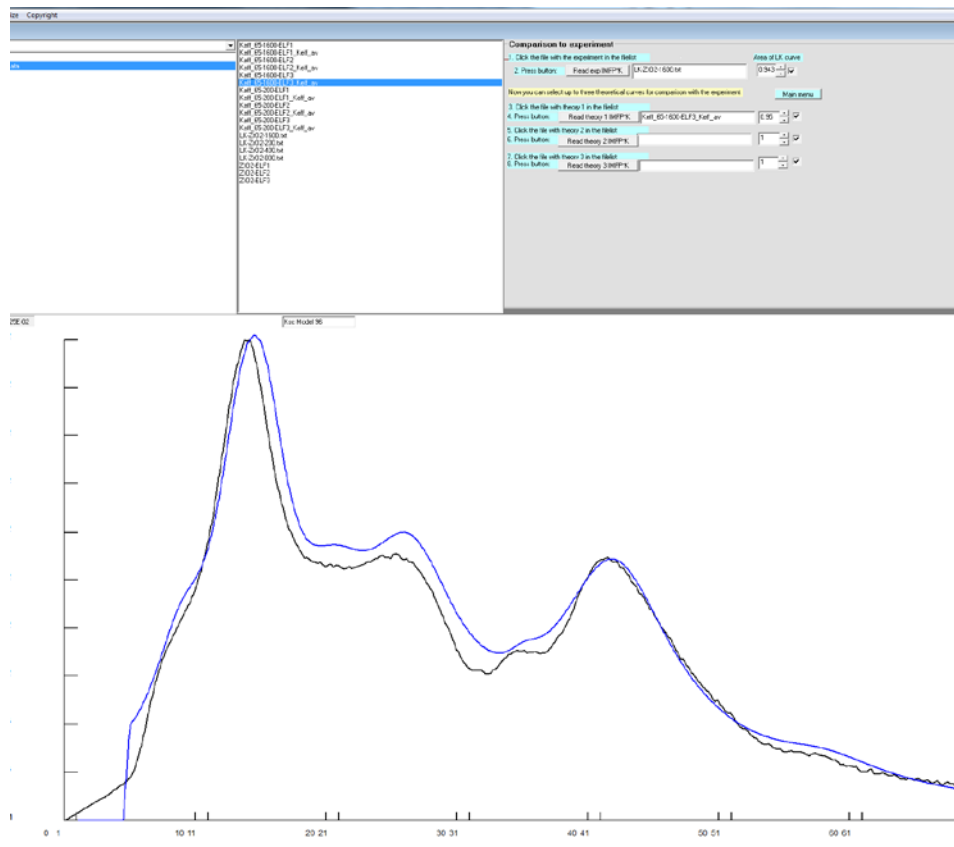


Fig.(15)

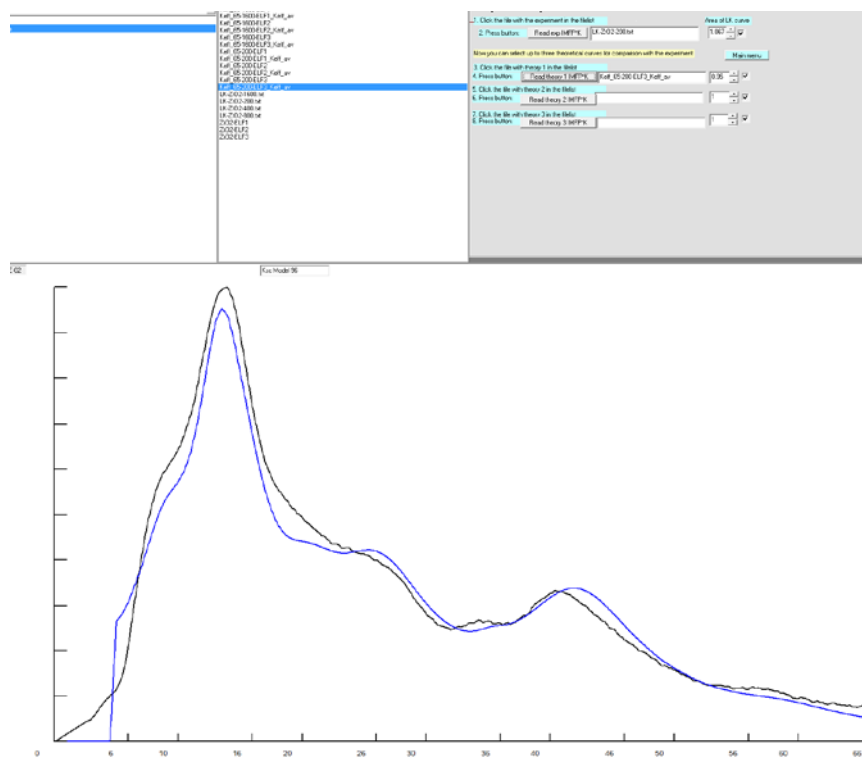


Fig.(16)

Fig. 17 shown the effect of using the parameters d_Gap and A_Gap with the values in table 4. This ELF is obtained in the *Set Oscillators* menu by first reading ZrO2-ELF3 (table3) and then setting the two parameters $d_Gap= 2.3$ and $A_Gap = 8$ and finally click *Auto Rescale Intensities A0 to fulfill KK-sum rule*.

The calculated cross section using this ELF, gives a better fit to experiment (See Fig.17) around the band gap energy. Note that the experimental cross section is by definition zero in the band gap region (i.e. < 4.5 eV) and that the fit should therefore only be looked for above the band gap energy.

Further small adjustments might be made now to improve the comparison a little. Likewise, one may use a finer energy grid and one might also include the spectra taken at 400 eV and 800 eV to fine adjust the oscillator parameters. This will not be done here.

Table 4:

The screenshot shows the 'ELF data' software interface. On the left is a table with columns 'w0', 'A0', 'g', and 'a'. The table contains 7 rows of data. To the right of the table are several control panels: 'File name' (ZrO2-ELF4), 'Band Gap' (E_Gap = 4.5, d_Gap = 2.3, A_Gap = 8), 'Number of oscillators = 7', 'Core excitations' (ac = 0.001, bc = -2), 'Check for KK-Sum Rule' (Material: Semicond/insulator, Input Refr. index = 1.9, KK-sum = 0.999999), and 'Plot ELF' (E_Max = 80, E_step = 0.2).

w0	A0	g	a
9.5	4.9979	5	0.05
15.2	62.443	4.5	0.05
21	35.429	6.5	0.05
26.7	126.61	8.5	0.05
35	7.1081	3	0.05
42	296.91	10	0.05
58	50.645	10	0.05

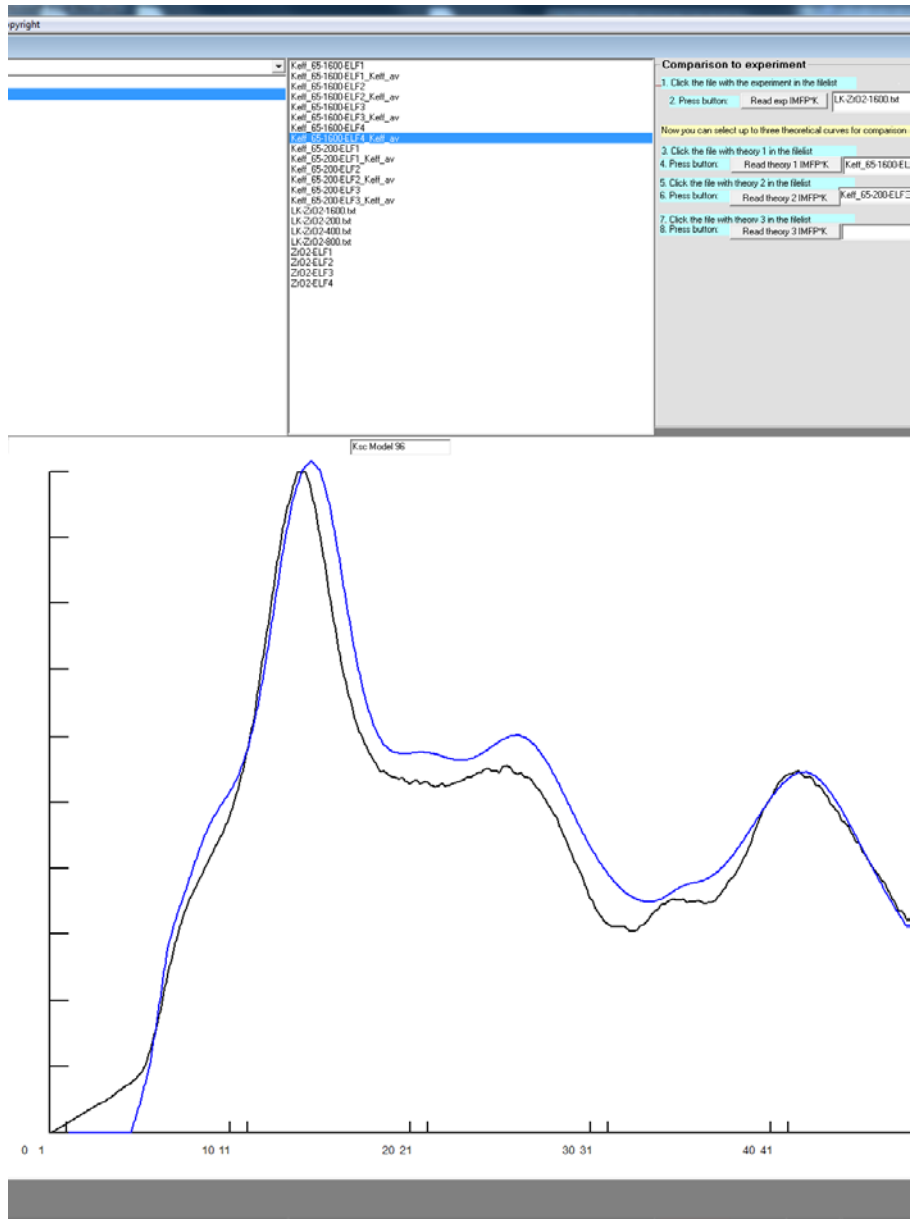


Fig. 17

The values in table 3 are slightly different from those previously reported in [10] obtained by analysis of the same experiment. The reason is that the calculations in [10] were done for normal incidence and exit angles while the present calculations were done for 60° incidence and normal emission angles which correspond to the situation in the experiment. The theory for general geometries was published in 1996 [6] while the previous analysis in [10] was done in 1994 based on the theory published in 1992 which is only for normal incidence and exit angles [5].

9.1.5 Calculation of optical properties

In the above steps the ELF for the material has been determined. It is now possible to calculate the optical properties of the solid in the form of the energy dependence of the real and imaginary parts of the dielectric function, the refractive index, the extinction coefficient and the absorption coefficient. This is done with the facilities in the menu: Calculate Optical Properties. To do that, open the menu and follow the instructions on the screen. See also Chapter 5.

From the main menu, select the menu *Calculate optical properties*. Click the file *ZrO2-ELF4* in the file list. Then click *Read ELF file* and get Fig. 18.

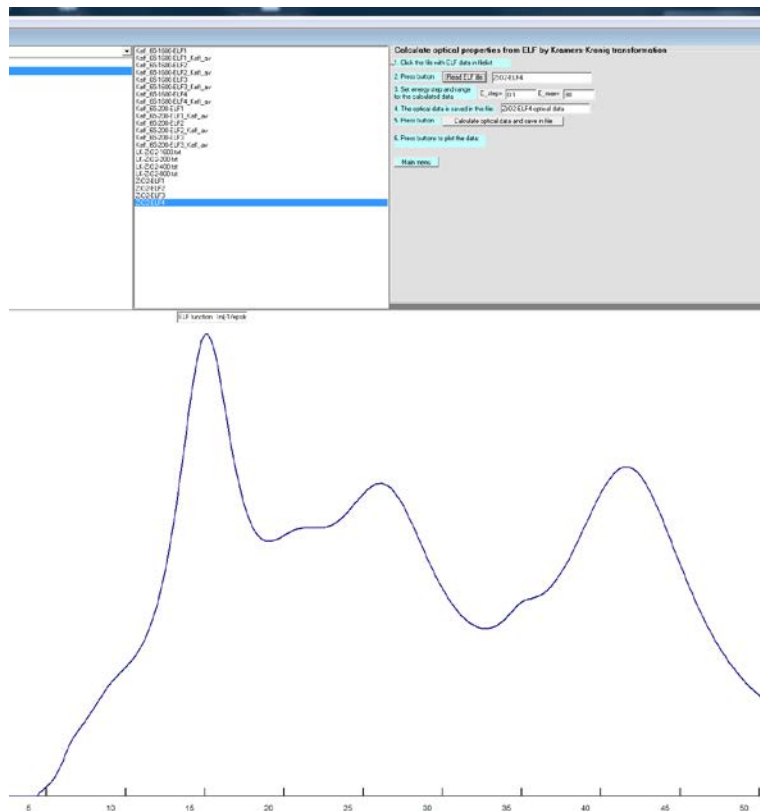


Fig. 18

Click the button *Calculate optical data and save in file*. This will start the calculation of the optical data which are saved in the file *ZrO2-ELF4-optical data* which now appears in the file-list. You can open this file to see the data. You plot the data by clicking *eps1*, *eps2* which are the real ϵ_1 and imaginary part ϵ_2 of the dielectric function $\epsilon = \epsilon_1 + i\epsilon_2$ (see figs. 19 and 20). The other optical data are plotted by clicking the corresponding buttons:

Fig. 21 shows the refractive index n

Fig. 22 the extinction coefficient k

Fig. 23 the absorption coefficient μ [μm^{-1}]

Fig. 24 the energy loss function $ELF = \text{Im}\left[\frac{-1}{\epsilon(0,\omega)}\right]$

Fig. 25 the surface energy loss function $SELF = \text{Im}\left[\frac{-1}{\epsilon(0,\omega)+1}\right]$

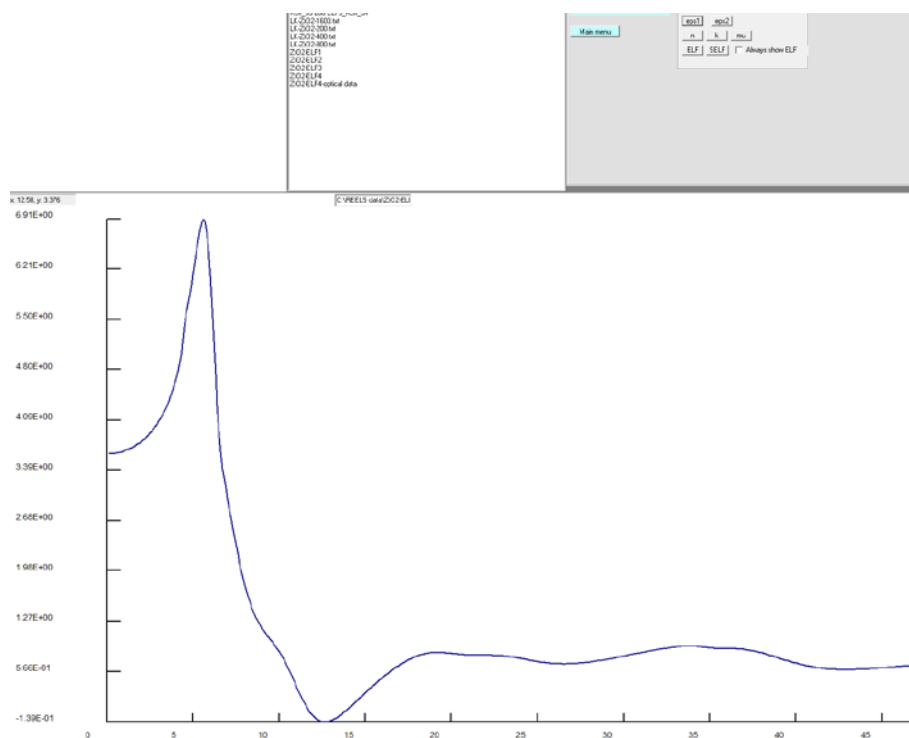


Fig. 19 ϵ_1

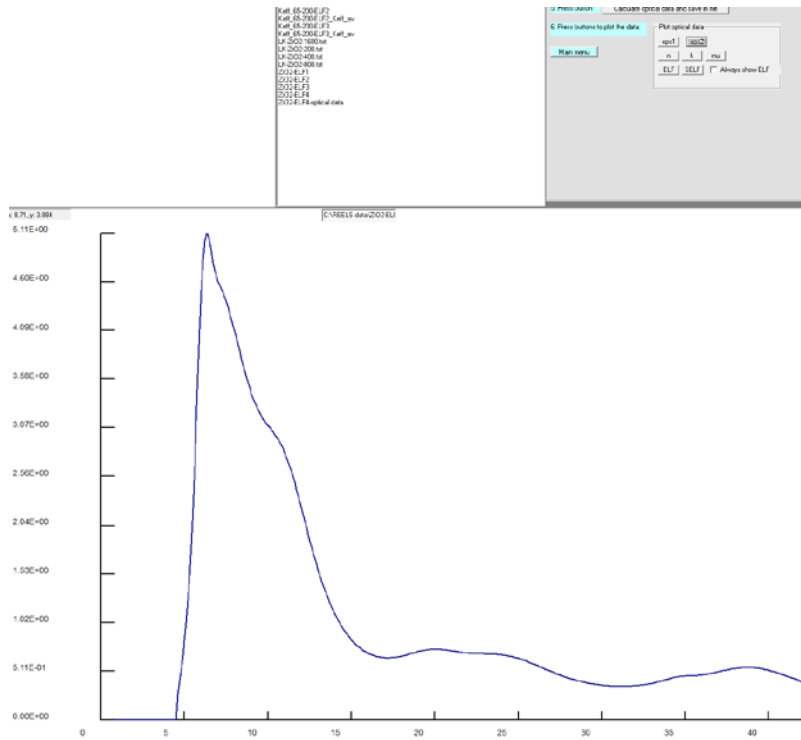


Fig. 20 ϵ_2

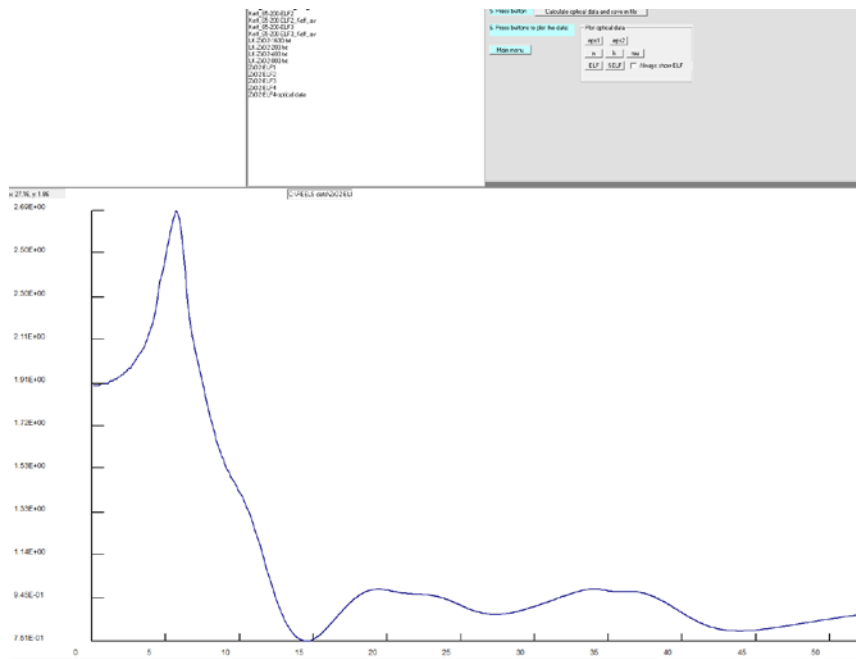


Fig. 21: the refractive index n

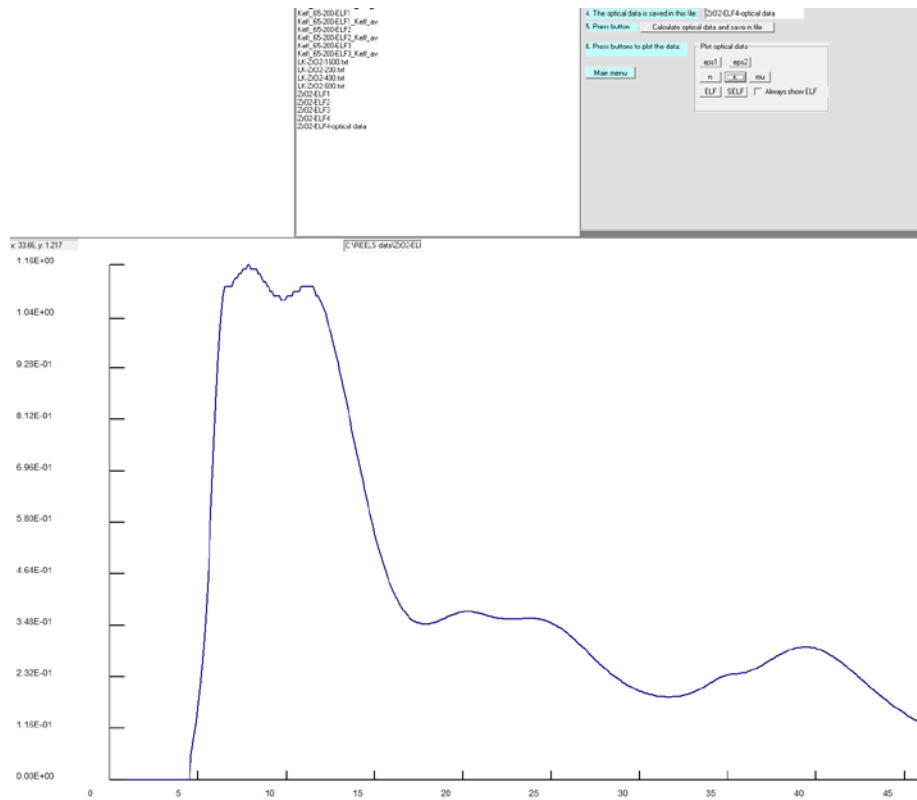


Fig. 22: the extinction coefficient k

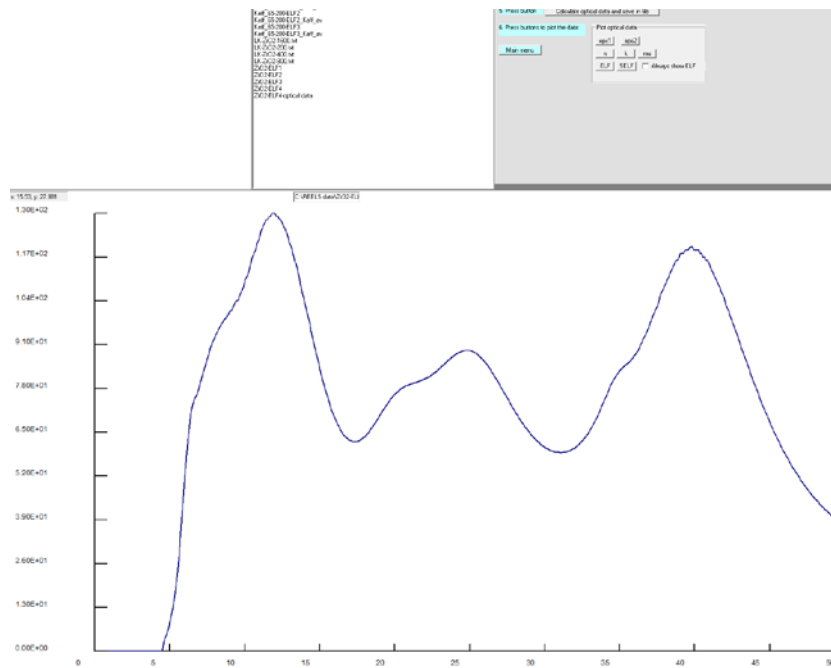


Fig. 23: the absorption coefficient μ [μm^{-1}].

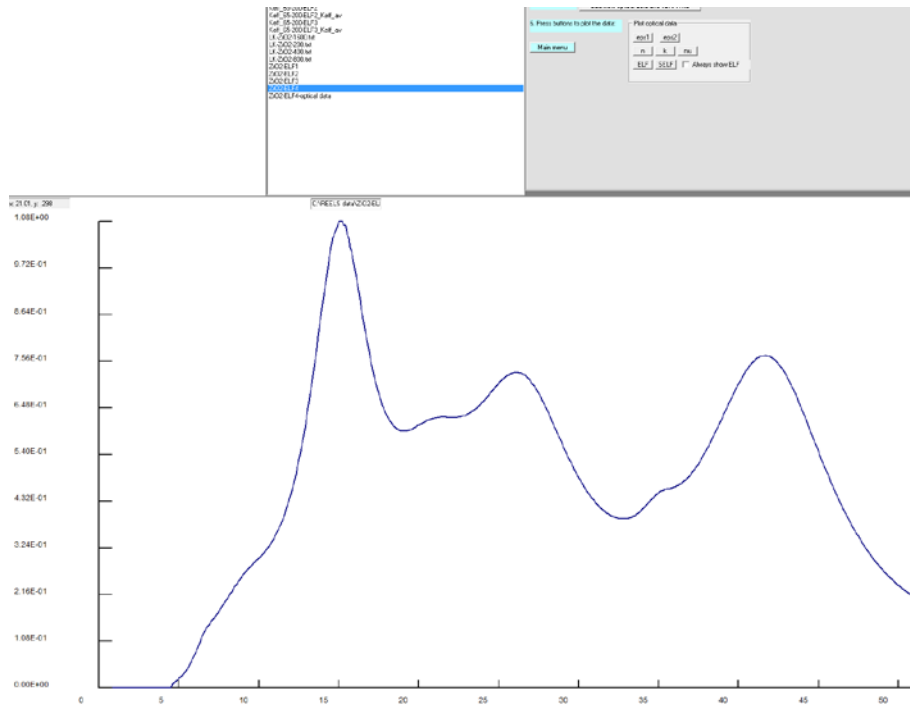


Fig. 24: the energy loss function $ELF = Im\left[\frac{-1}{\varepsilon(0,\omega)}\right]$

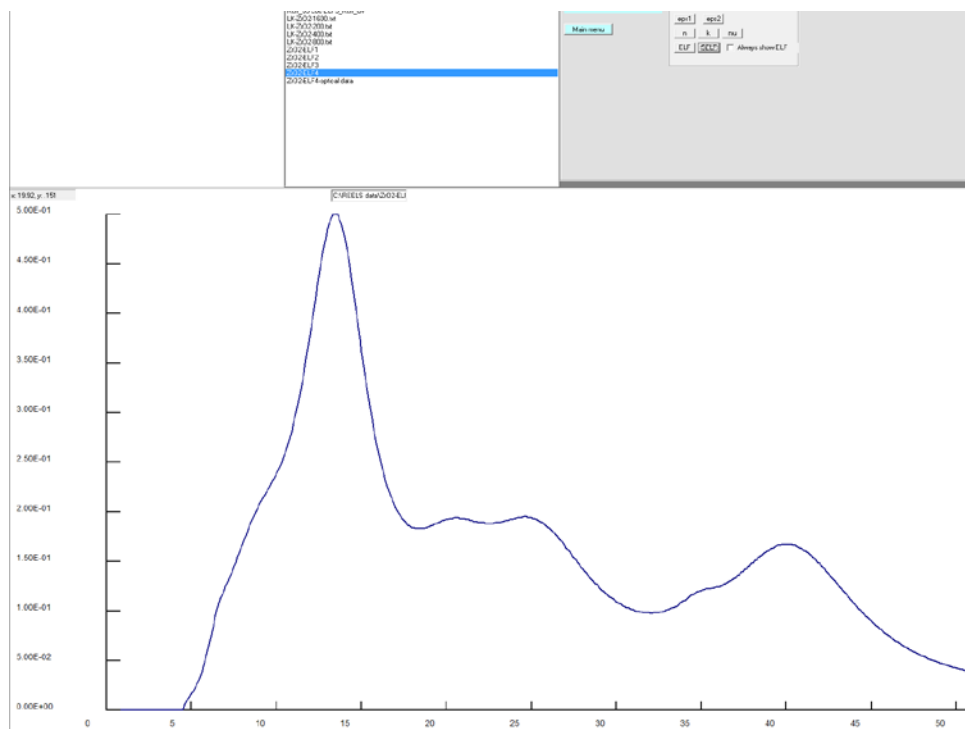


Fig. 25: the surface energy loss function $SELF = Im\left[\frac{-1}{\varepsilon(0,\omega)+1}\right]$

10. 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 required data format.

To facilitate these operations, a file management system is included.

It appears in the upper left part of the screen and 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 different 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.

You cannot delete or move files. To do this, use the Windows file management system.

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.

10.1 File Formats.

QUASES_XS_REELS_1 uses the QUASES-standard data format.

This data 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.

11. Smooth.

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

Click **Smooth Spectra**.

Click the filename with the spectrum in the *Filelist* .

Both the unsmoothed and the smoothed spectra may be plotted by clicking the check box. Use this to judge the degradation of sharp features 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:
change the values of

Number of points ns
and

Order m of polynomial fit

A moderate smoothening which does not degrade the structure in the spectra is usually obtained with $ns = 3$ and $m = 2$ which are recommended default values.

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 different name.

Click **Save Spectrum**.

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

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QUEELS- $\epsilon(k,\omega)$ -REELS