Software Package to Calculate the Effects of Core hole and Surface Excitations on XPS and AES

Sven Tougaard , Francisco Yubero

QUEELS-XPS software package
Semi-classical dielectric response model

1. Intro: REELS Semi-classical dielectric response model

2. The XPS- Semiclassical dielectric response model
   Intrinsic and extrinsic excitations

3. The QUEELS-XPS software package

4. The validity of the model
   quantitative comparison with experiments

1. Intro: REELS Semi-classical dielectric response model
   QUEELS-ε(k,ω)-REELS software package

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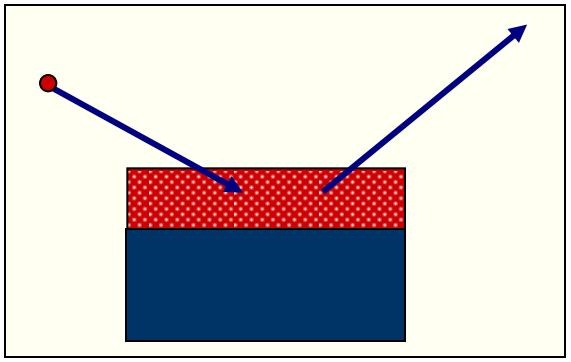
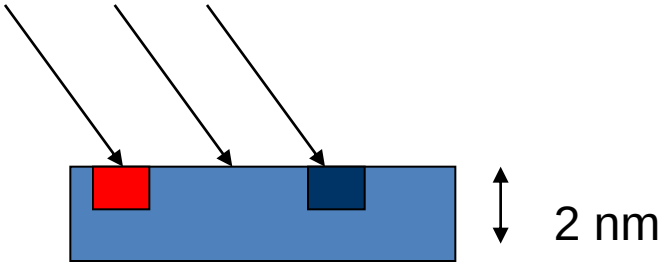
Dielectric response model for REELS

Tougaard and Chorkendorff Phys Rev B35, 6570 (1987)
Yubero and Tougaard Phys Rev B46, 2486 (1992)
Yubero, Sanz, Ramskov, Tougaard Phys Rev B53, 9719 (1996)





Low energies are necessary

Surface effects and k-dispersion effects are important

Quantitative determination of

dielectric function

optical properties

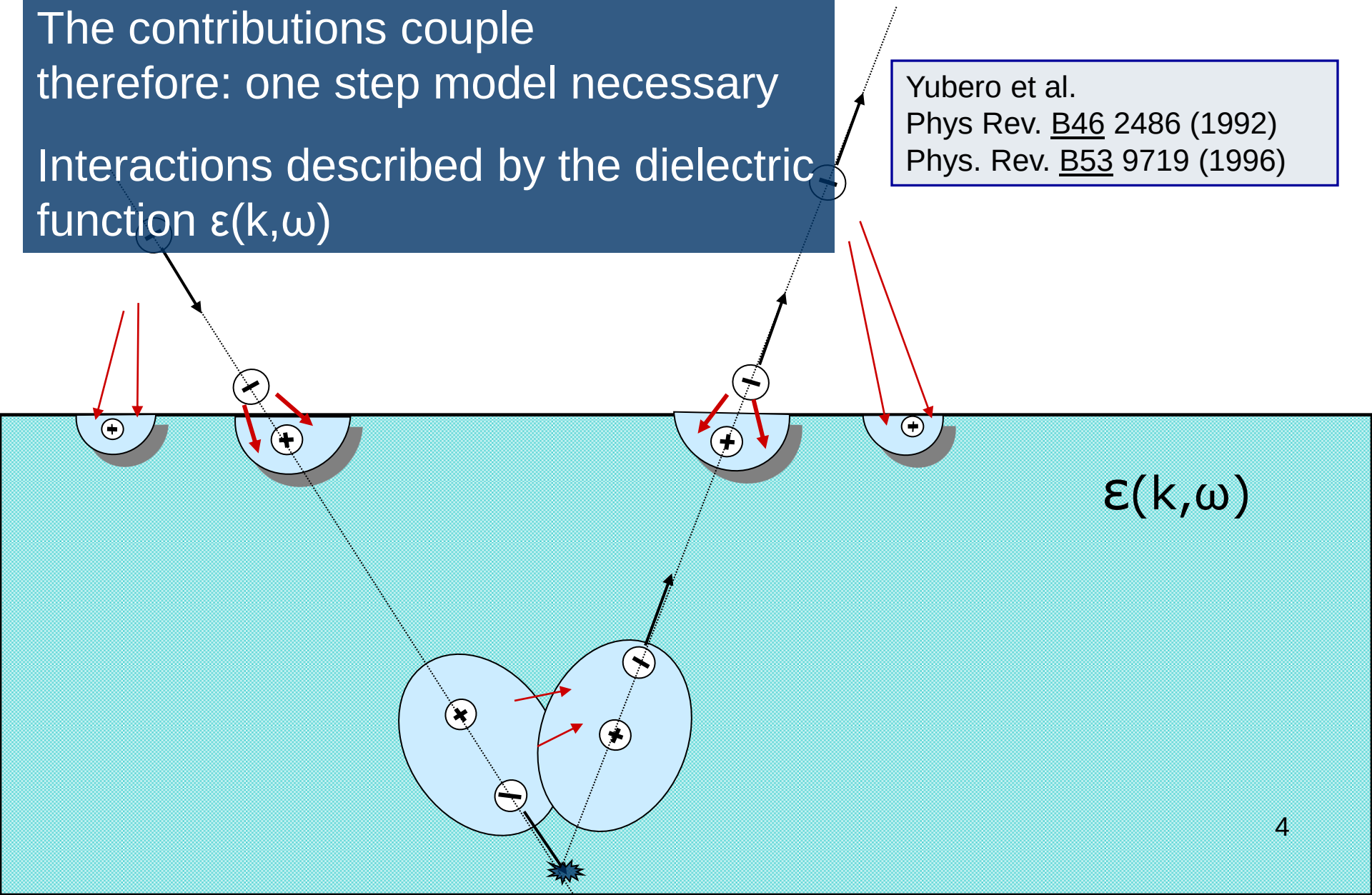
of nano-meter thin films

Semiclassical dielectric response model for REELS

The contributions couple
therefore: one step model necessary

Interactions described by the dielectric function ε(k,ω)

Yubero et al.
Phys Rev. B46 2486 (1992)
Phys. Rev. B53 9719 (1996)



Effective cross section

ε(k,ω) is the only unknown

Compare model calculation to REELS-experiment

Determination of the dielectric function ε(k,ω)

QUEELS- ε(k,ω)-REELS software was developed to easily do this

Each term can be found from the following expressions:

$$\left.\delta(k_\perp-\Omega_i)-i\,\frac{e^{-i(k_\perp-\Omega_i)a}}{k_\perp-\Omega_i}\right]\Bigg\}, \tag{17}$$

$$K_{\rm eff}^{M_i}=\mathrm{Re}\left\{\frac{-2ie}{(2\pi)^4\hbar^2\omega x}\int d\mathbf{k}\left(k_\perp+k_\parallel\frac{v_{\parallel i}^*}{v_{\perp i}}\right)e^{ik_\perp a}\Phi_{\rm ind}^M(\mathbf{k},\omega)\left[\frac{1-e^{-i(k_\perp-\Omega_i)a}}{k_\perp-\Omega_i}\right]\right\}, \tag{18}$$

$$K_{\rm eff}^{V_o}=\mathrm{Re}\left\{\frac{-2ie}{(2\pi)^4\hbar^2\omega x}\int d\mathbf{k}\left(k_\perp-k_\parallel\frac{v_{\parallel o}}{v_{\perp o}}\right)e^{ik_\perp a}\Phi_{\rm ind}^V(\mathbf{k},\omega)\left[\pi\delta(k_\perp+\Omega_o)-i\,\frac{e^{-i(k_\perp+\Omega_o)a}}{k_\perp+\Omega_o}\right]\right\}, \tag{19}$$

$$K_{\rm eff}^{M_o}=\mathrm{Re}\left\{\frac{2e}{(2\pi)^4\hbar^2\omega x}\int d\mathbf{k}\left(k_\perp-k_\parallel\frac{v_{\parallel o}}{v_{\perp o}}\right)e^{ik_\perp a}\Phi_{\rm ind}^M(\mathbf{k},\omega)\left[\frac{1-e^{-i(k_\perp+\Omega_o)a}}{k_\perp+\Omega_o}\right]\right\}. \tag{20}$$

Equations (16)–(20) give the solution to the problem of finding $K_{\rm eff}$ for a general REELS geometry. However, in the following we will consider approximations that allow some integrals to be done analytically.

The integrals in momentum are given by the conservation laws for energy and momentum. Unfortunately a complete analytical integration is not possible. However, with cylindrical coordinates ($d\mathbf{k}=2\pi dk_\parallel dk_\perp$) and extending the limits of integration over $k_\perp$ to $-\infty<k_\perp<+\infty$, the integral over $k_\perp$ can be done analytically. With this approximation we do not expect large errors because the main contribution to the integral comes from small values of k, and the integrand decreases roughly as $1/k^9$ for $k\to\pm\infty$ using the functional shape for the ELF as in Eq. (30) (see below). Assuming again $\epsilon=\epsilon(k_\parallel,\omega)$, it is found that

$$K_{\rm eff}^{V_i}=\mathrm{Re}\left\{\frac{e}{\hbar^2\omega\pi x}\frac{v_{\perp i}+iv_{\parallel i}}{v_{\perp i}}\int dk_\parallel\,\frac{\epsilon-1}{\epsilon+1}\frac{k_\parallel(k_\parallel+i\Omega_i)}{k_\parallel^2+\Omega_i^2}\,e^{i\Omega_i a}[F^{MM}(k_\parallel)+F^{MV}(k_\parallel)]\right\}, \tag{21}$$

$$K_{\rm eff}^{V_o}=\mathrm{Re}\left\{\frac{-e}{\hbar^2\omega\pi x}\frac{v_{\perp o}-iv_{\parallel o}}{v_{\perp o}}\int dk_\parallel\,\frac{\epsilon-1}{\epsilon+1}\frac{k_\parallel(k_\parallel-i\Omega_o)}{k_\parallel^2+\Omega_o^2}\,e^{-i\Omega_o a}[F^{MM}(k_\parallel)+F^{MV}(k_\parallel)]\right\}, \tag{22}$$

$$\begin{aligned}K_{\rm eff}^{M_i}=&\mathrm{Re}\left\{\frac{-2ie^2}{\hbar^2\pi v_{\perp i}^2}\frac{a}{x}\int dk_\parallel\left(\frac{1}{\epsilon}-1\right)\frac{k_\parallel}{k_\parallel^2+\Omega_i^2}\right\}+\mathrm{Re}\left\{\frac{-2e^2}{\hbar^2\pi v_{\perp o}\omega x}\int dk_\parallel\left(\frac{1}{\epsilon}-1\right)\frac{e^{i(\Omega_i+\Omega_o)}-1}{\Omega_i+\Omega_o}\frac{k_\parallel}{k_\parallel^2+\Omega_o^2}\left[k_\parallel\left(\frac{v_{\parallel i}}{v_{\perp i}}+\frac{v_{\parallel o}}{v_{\perp o}}\right)\right.\right.\\&\left.\left.-\frac{\omega}{v_{\perp o}}\right]\right\}+\mathrm{Re}\left\{\frac{e}{\hbar^2\pi\omega x}\frac{v_{\perp i}-iv_{\parallel i}}{v_{\perp i}}\int dk_\parallel\left(\frac{1}{\epsilon}-1\right)\frac{k_\parallel(k_\parallel-i\Omega_i)}{k_\parallel^2+\Omega_i^2}\,(e^{-k_\parallel a}-e^{i\Omega_i a})\rho_1^M(k_\perp=ik_\parallel)\right\}\\&+\mathrm{Re}\left\{\frac{e}{\hbar^2\pi\omega x}\frac{v_{\perp i}+iv_{\parallel i}}{v_{\perp i}}\int dk_\parallel\left(\frac{1}{\epsilon}-1\right)\frac{k_\parallel(k_\parallel+i\Omega_i)}{k_\parallel^2+\Omega_i^2}\,(e^{k_\parallel a}-e^{i\Omega_i a})\rho_2^M(k_\perp=-ik_\parallel)\right\}\\&+\mathrm{Re}\left\{\frac{e}{\hbar^2\pi^2\omega x}\frac{v_{\perp i}-iv_{\parallel i}}{2v_{\perp i}}\int dk_\parallel\left[\frac{(\epsilon+2)(\epsilon-1)}{\epsilon(\epsilon+1)}F^{MM}(k_\parallel)-\frac{\epsilon-1}{\epsilon+1}F^{MV}(k_\parallel)\right]\frac{k_\parallel(k_\parallel-i\Omega_i)}{k_\parallel^2+\Omega_i^2}\,(e^{-k_\parallel a}-e^{i\Omega_i a})\right\},\end{aligned} \tag{23}$$

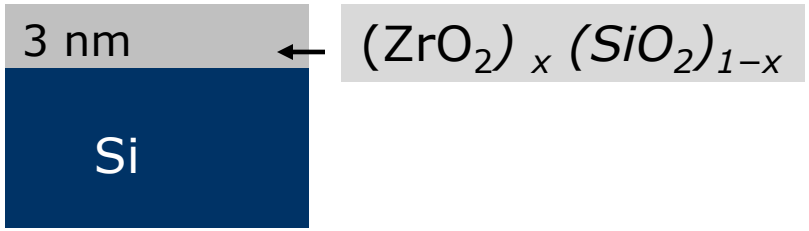
$$\begin{aligned}K_{\rm eff}^{M_o}=&\mathrm{Re}\left\{\frac{-2ie^2}{\hbar^2\pi v_{\perp o}^2}\frac{a}{x}\int dk_\parallel\left(\frac{1}{\epsilon}-1\right)\frac{k_\parallel}{k_\parallel^2+\Omega_o^2}\right\}+\mathrm{Re}\left\{\frac{2e^2}{\hbar^2\pi v_{\perp i}\omega x}\int dk_\parallel\left(\frac{1}{\epsilon}-1\right)\frac{e^{-i(\Omega_i+\Omega_o)}-1}{\Omega_i+\Omega_o}\frac{k_\parallel}{k_\parallel^2+\Omega_i^2}\left[k_\parallel\left(\frac{v_{\parallel i}}{v_{\perp i}}+\frac{v_{\parallel o}}{v_{\perp o}}\right)\right.\right.\\&\left.\left.-\frac{\omega}{v_{\perp i}}\right]\right\}+\mathrm{Re}\left\{\frac{-e}{\hbar^2\pi\omega x}\frac{v_{\perp o}+iv_{\parallel o}}{v_{\perp o}}\int dk_\parallel\left(\frac{1}{\epsilon}-1\right)\frac{k_\parallel(k_\parallel+i\Omega_o)}{k_\parallel^2+\Omega_o^2}\,(e^{-k_\parallel a}-e^{-i\Omega_o a})\rho_1^M(k_\perp=ik_\parallel)\right\}\\&+\mathrm{Re}\left\{\frac{-e}{\hbar^2\pi\omega x}\frac{v_{\perp o}-iv_{\parallel o}}{v_{\perp o}}\int dk_\parallel\left(\frac{1}{\epsilon}-1\right)\frac{k_\parallel(k_\parallel-i\Omega_o)}{k_\parallel^2+\Omega_o^2}\,(e^{k_\parallel a}-e^{-i\Omega_o a})\rho_2^M(k_\perp=-ik_\parallel)\right\}\\&+\mathrm{Re}\left\{\frac{-e}{\hbar^2\pi^2\omega x}\frac{v_{\perp o}+iv_{\parallel o}}{2v_{\perp o}}\int dk_\parallel\left[\frac{(\epsilon+2)(\epsilon-1)}{\epsilon(\epsilon+1)}F^{MM}(k_\parallel)-\frac{\epsilon-1}{\epsilon+1}F^{MV}(k_\parallel)\right]\frac{k_\parallel(k_\parallel+i\Omega_o)}{k_\parallel^2+\Omega_o^2}\,(e^{-k_\parallel a}-e^{-i\Omega_o a})\right\}.\end{aligned} \tag{24}$$

Notice that $K_{\rm eff}^{V_o,M_o}$ can be obtained from $K_{\rm eff}^{V_iM_i}$ by making the changes $v_{\perp o}\to-v_{\perp i}$, $v_{\perp j}\to-v_{\perp o}$, $v_{\parallel i}\to v_{\parallel o}$, and $v_{\parallel o}\to v_{\parallel i}$. Note also that in general $K_{\rm eff}(E_0,\hbar\omega,a,\theta_o,\theta_o)\neq K_{\rm eff}(E_0,\hbar\omega,a,\theta_0,\theta_i)$, i.e., the losses experienced by the electron depend not only on the line trajectory followed but also on the sense in which it is done. However, in practice the difference is very small.

We must discuss now the limits in which the present model can be compared with model B in Ref. 9. That model is valid for normal incidence and exit angles of the electrons. This situation is given in the present model by considering $v_{\parallel i}=v_{\parallel o}=0$ and $v_{\perp i}=v_{\perp o}=v$, which gives

Application to Si-gate oxides

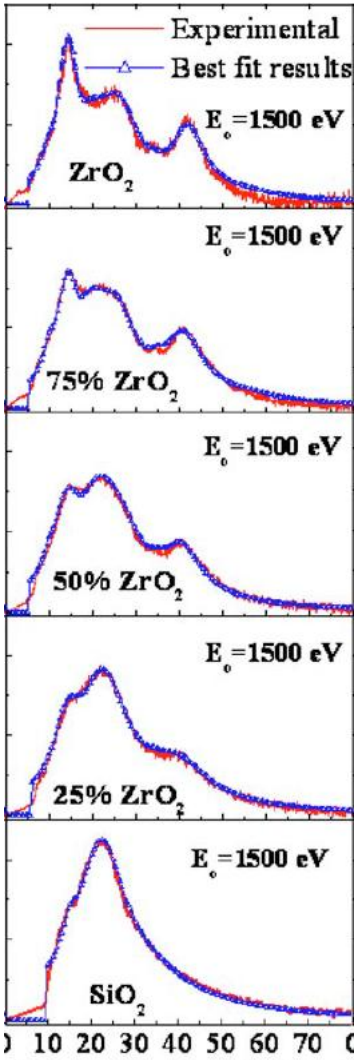
Tahir et al. J. Appl. Phys 106 (2009) 084108

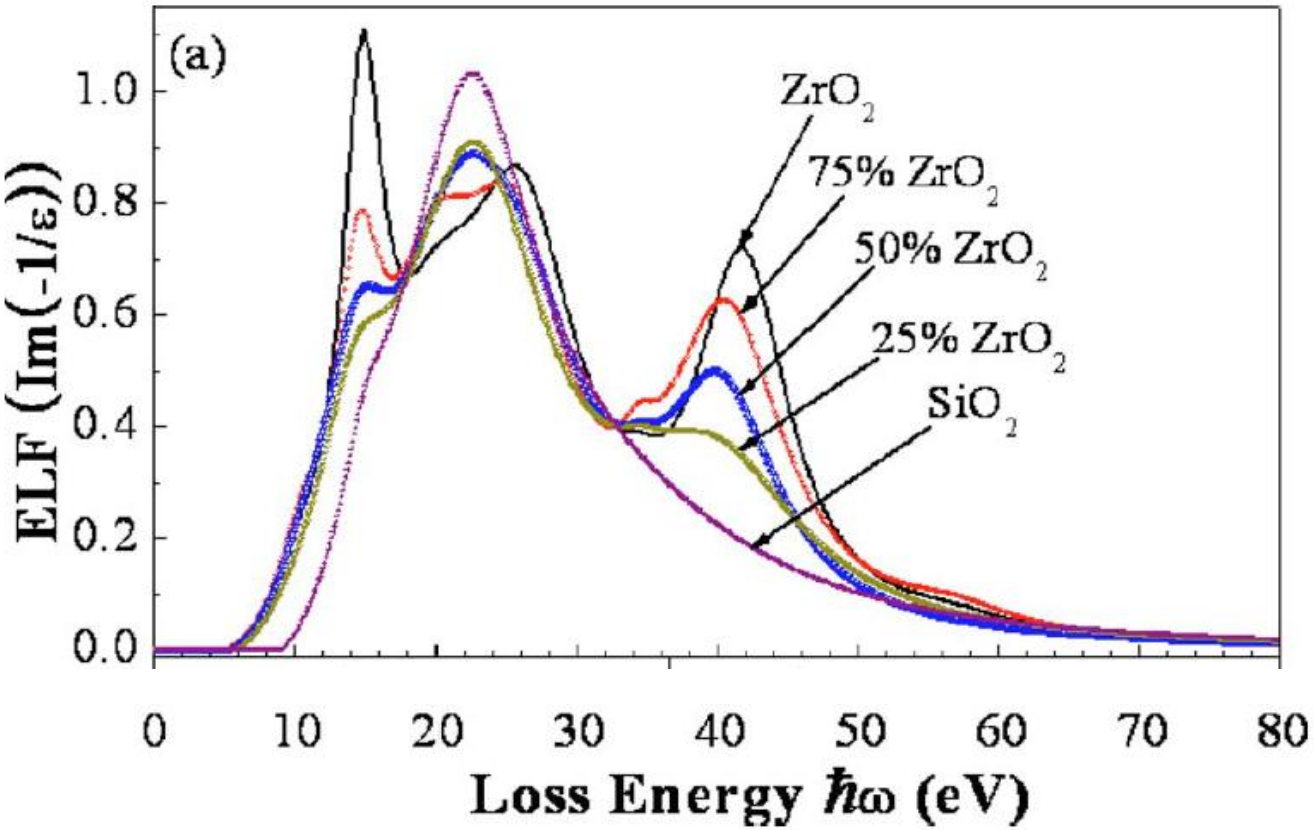


REELS exp comp to theory

Im [-1/ε(k,ω)]

$(ZrO_2)_x (SiO_2)_{1-x}$



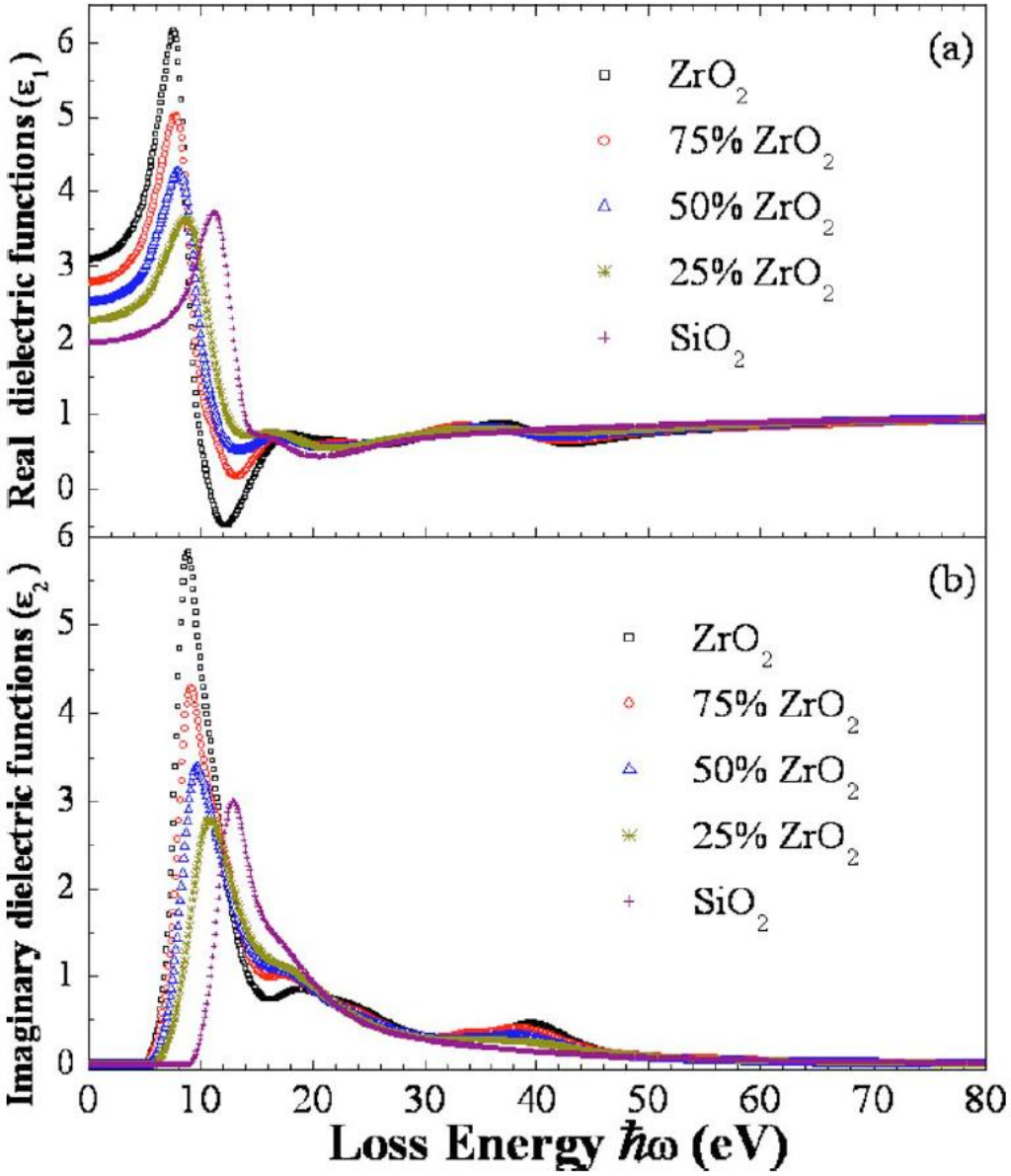


Tahir et al. J. Appl. Phys 106 (2009) 084108

$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$

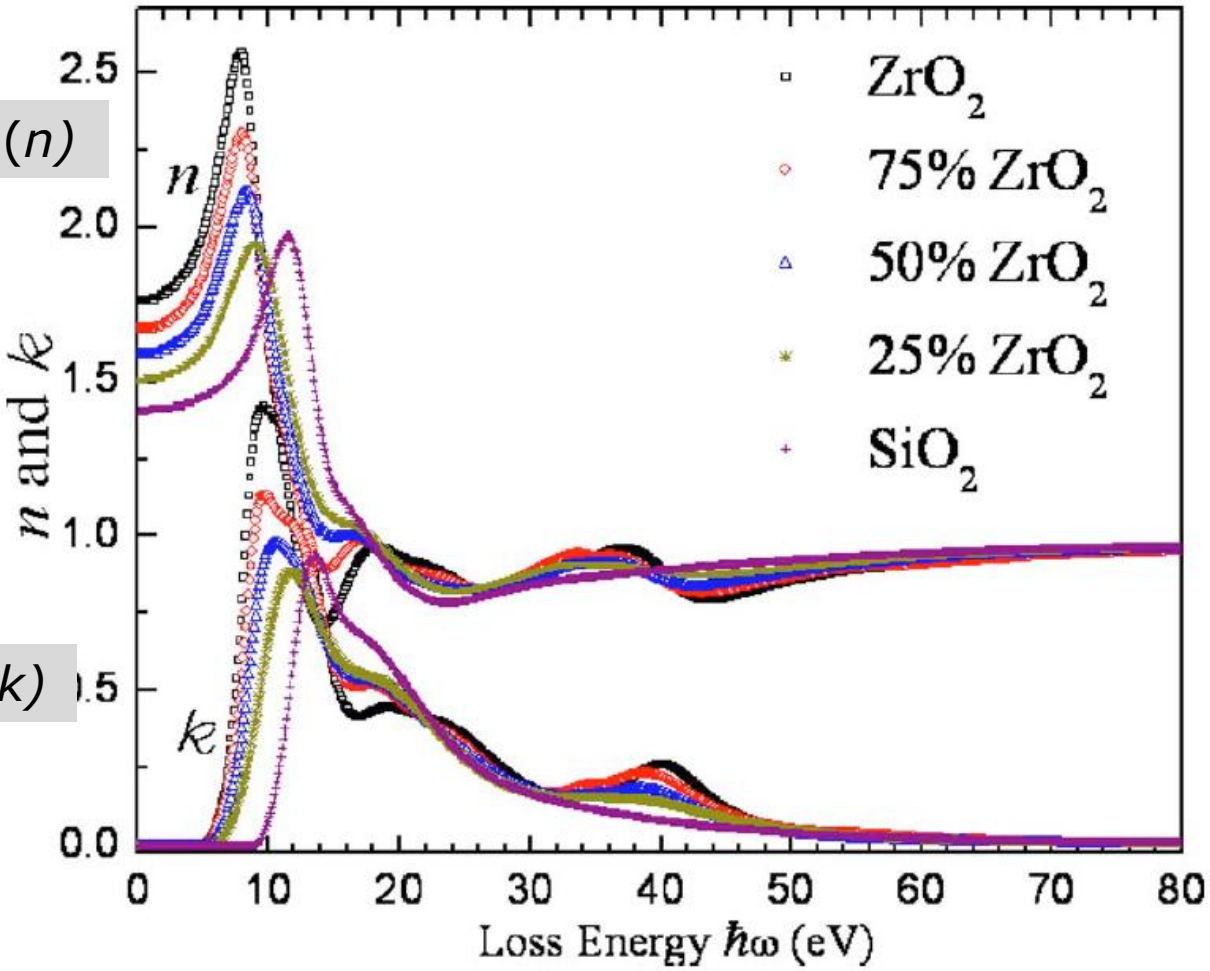
$\varepsilon_1(\omega)$

$\varepsilon_2(\omega)$



Index of refraction (*n*)

Extinction coefficient (*k*)



QUEELS- ε(k,ω)-REELS software package

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QUEELS-XPS software package
Semi-classical dielectric response model

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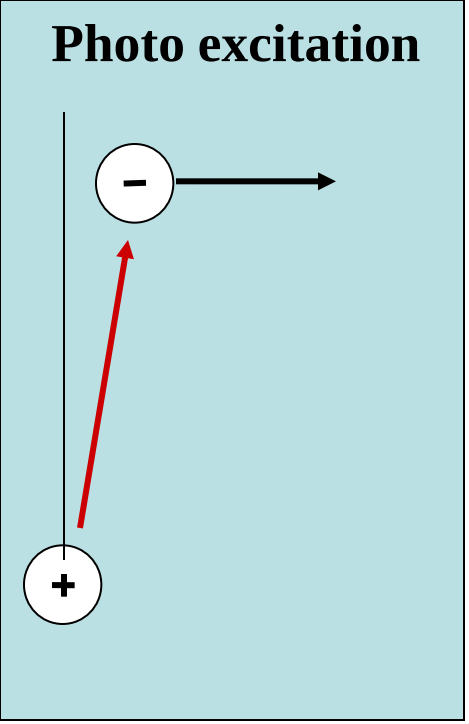
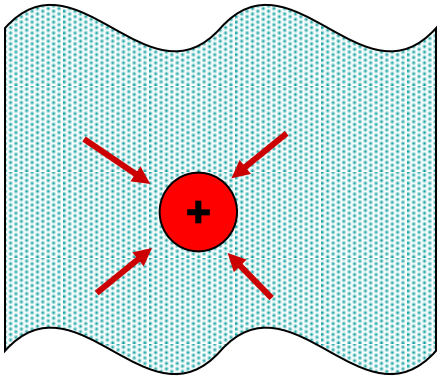


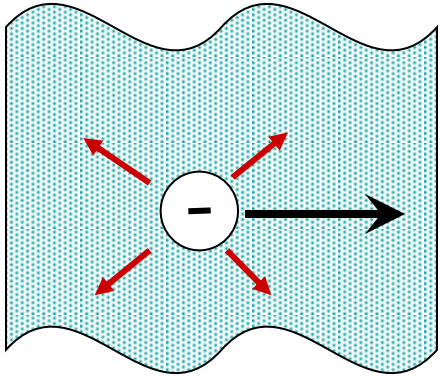
Intrinsic and extrinsic excitations:



Sudden creation of a core hole

Intrinsic Shake-up excitations

+



Moving electron

Extrinsic Energy loss

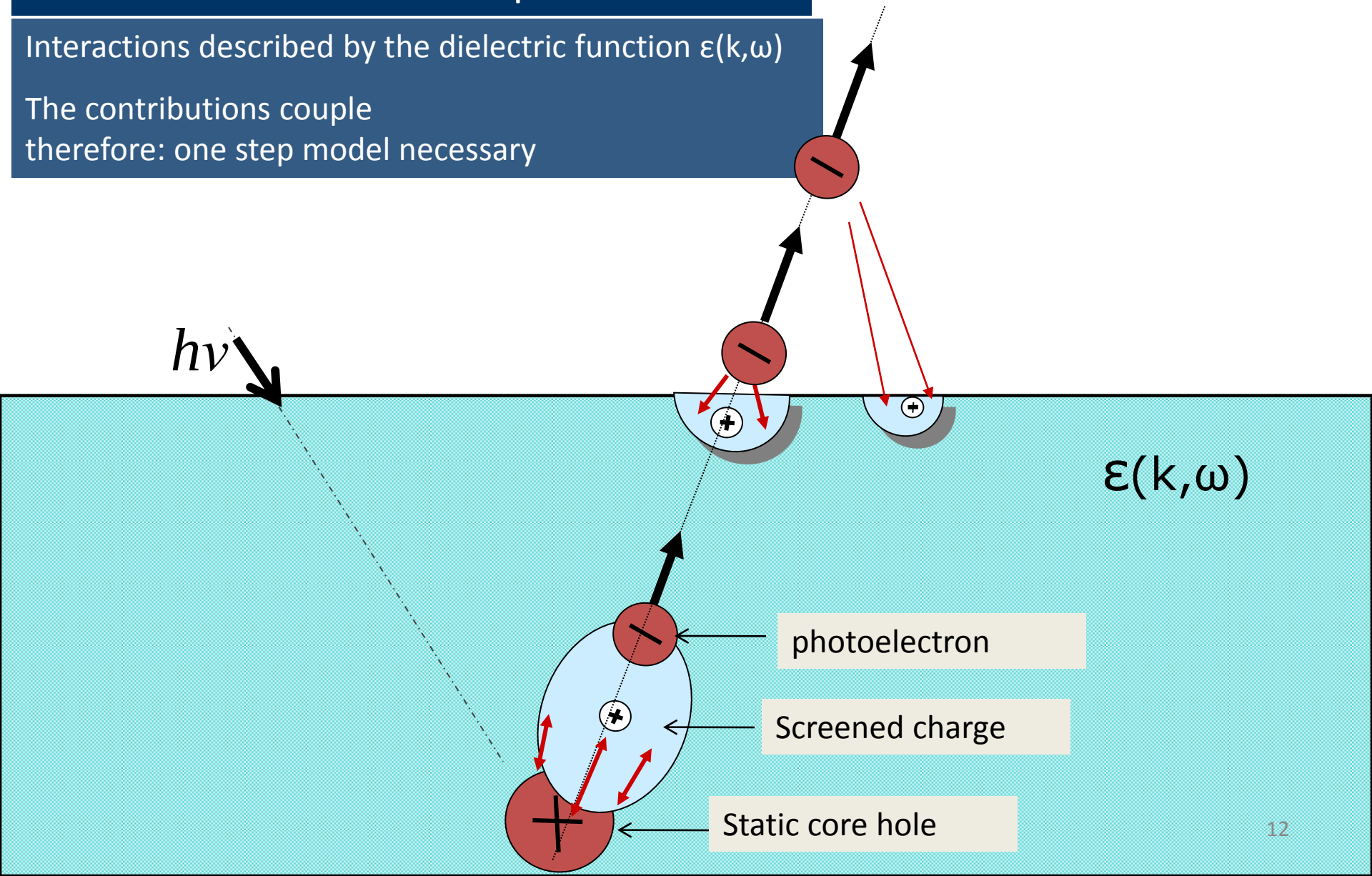
The contributions interfere and cannot be separated

XPS
Semiclassical dielectric response model

Phys. Rev.B56 (1997)1612

Interactions described by the dielectric function ε(k,ω)

The contributions couple
therefore: one step model necessary



Effective cross section

$$K_{eff}=K_{M1}+K_{M2}+K_{M3}+K_V$$

$$K_{M1}=\frac{\cos\theta}{\pi a_0 E_\perp}\,\mathrm{Re}\left[i\int k_\parallel dk_\parallel \frac{(1/\epsilon-1)}{\Omega_0^2+k_\parallel^2}\right]+\frac{-1}{2\pi E_\perp a_0 x\omega_\perp}\,\mathrm{Re}\left[i\int k_\parallel dk_\parallel \frac{(1/\epsilon-1)}{(\Omega_0^2+k_\parallel^2)^2}\left\{\left(i+\frac{\nu_\parallel}{\nu_\perp}\right)(\Omega_0+ik_\parallel)^2(e^{-i\Omega_0 a-k_\parallel a}-1)\right.\right.$$
$$\left.\left.+\left(-i+\frac{\nu_\parallel}{\nu_\perp}\right)(\Omega_0-ik_\parallel)^2(e^{i\Omega_0 a-k_\parallel a}-1)+\left(i-\frac{\nu_\parallel}{\nu_\perp}\right)(e^{-i\Omega_0 a}-e^{-k_\parallel a})(e^{i\Omega_0 a}-e^{-k_\parallel a})(\Omega_0^2+k_\parallel^2)\right\}\right], \quad (13)$$

$$K_{M2}=\frac{-1}{2\pi E_\perp a_0 x\omega_\perp}\,\mathrm{Re}\left[\left(\pi\delta(\omega_\perp)+\frac{i}{\omega_\perp}\right)\int k_\parallel dk_\parallel \frac{(1/\epsilon-1)}{\Omega_0^2+k_\parallel^2}\left\{\left(i+\frac{\nu_\parallel}{\nu_\perp}\right)(\Omega_0+ik_\parallel)(1-e^{-k_\parallel a-i\Omega_0 a})\right.\right.$$
$$\left.\left.+\left(-i+\frac{\nu_\parallel}{\nu_\perp}\right)(\Omega_0-ik_\parallel)(e^{-2k_\parallel a}-e^{-k_\parallel a-i\Omega_0 a})\right\}\right], \quad (14)$$

$$K_{M3}=\frac{-1}{2\pi E_\perp a_0 x\omega_\perp}\,\mathrm{Re}\left[i\int k_\parallel dk_\parallel \frac{(-i+\nu_\parallel/\nu_\perp)(\Omega_0-ik_\parallel)(e^{-k_\parallel a}-e^{-i\Omega_0 a})}{\Omega_0^2+k_\parallel^2}\left\{\frac{(\epsilon-1)(\epsilon+2)}{\epsilon(\epsilon+1)}\left[(e^{i\Omega_0 a}-e^{-k_\parallel a})\left(\frac{\Omega_0+ik_\parallel}{\Omega_0^2+k_\parallel^2}\right)\right.\right.\right.$$
$$\left.\left.\left.-i\left(\pi\delta(\omega_\perp)+\frac{i}{\omega_\perp}\right)e^{-k_\parallel a}\right]+\frac{(\epsilon-1)}{(\epsilon+1)}\left(\frac{\Omega_0-ik_\parallel}{\Omega_0^2+k_\parallel^2}\right)e^{i\Omega_0 a}\right\}\right], \quad (15)$$

$$K_V=\frac{1}{2\pi E_\perp a_0 x\omega_\perp}\,\mathrm{Re}\left[\int k_\parallel dk_\parallel \frac{(1-\epsilon)}{(1+\epsilon)}\frac{(1-i\nu_\parallel/\nu_\perp)(\Omega_0+ik_\parallel)e^{-i\Omega_0 a}}{\Omega_0^2+k_\parallel^2}\left\{\frac{2ik_\parallel e^{i\Omega_0 a}-(\Omega_0+ik_\parallel)e^{-k_\parallel a}}{\Omega_0^2+k_\parallel^2}\right.\right.$$
$$\left.\left.-i\left(\pi\delta(\omega_\perp)+\frac{i}{\omega_\perp}\right)e^{-k_\parallel a}\right\}\right],$$

$\varepsilon(k,\omega)$ is the only unknown

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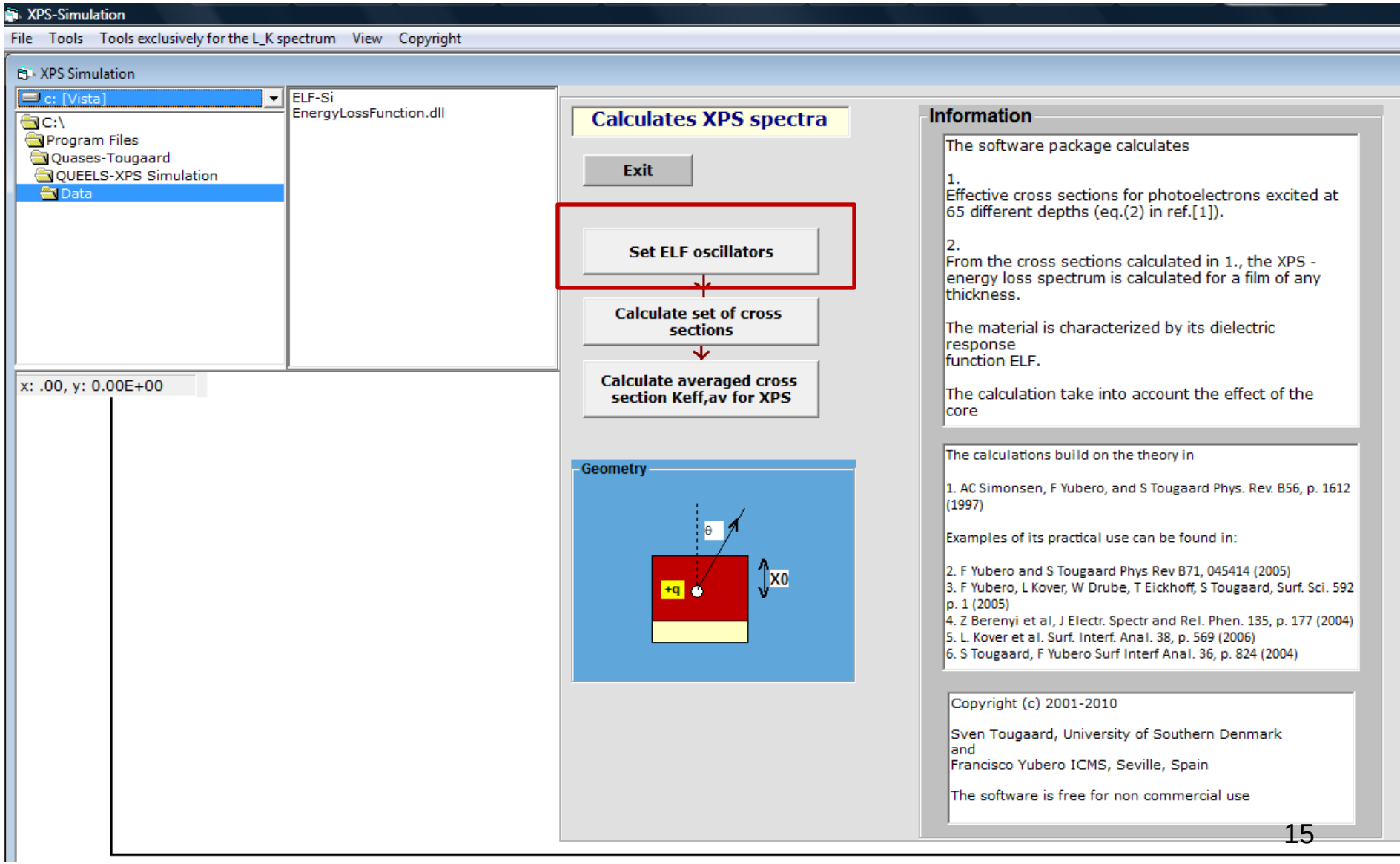
QUEELS-XPS software



XPS-Simulation

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XPS Simulation

c: [Vista]

C:\
Program Files
Quases-Tougaard
QUEELS-XPS Simulation
Data

ELF-Si
EnergyLossFunction.dll

ELF data

w0	A0	g	a
10	6	5	0.5
14	30	5	0.5
16.8	210	3.8	0.5

File name: ELF-Si

Read Save

Sort osc E_Gap = 0

Number of oscillators = 3

Core excitations
ac = 0.001
bc = -2

Main menu

Check for KK-Sum Rule
Refr. index = 4.5
KK-sum = 1.00649

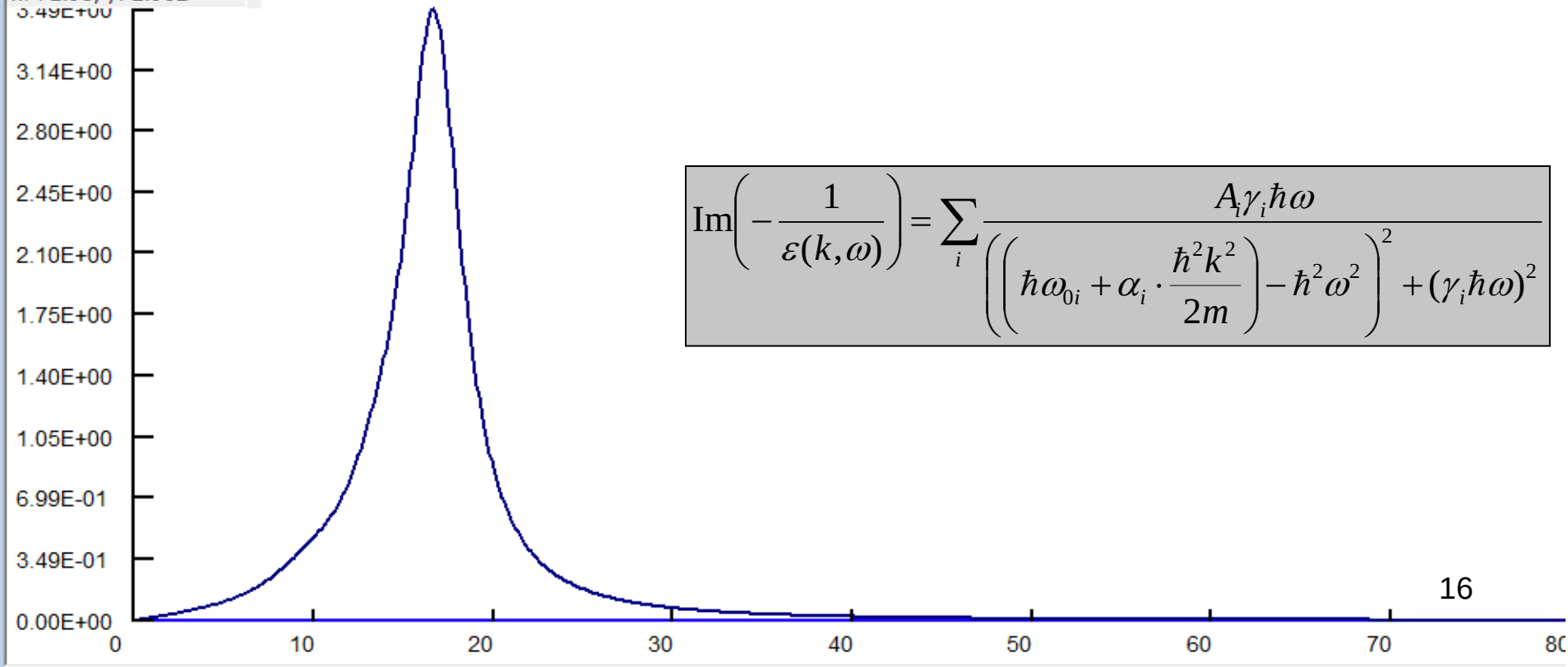
Typical Refr.Index values

Auto Rescale Intnsities A0 to fulfill KK-sum rule

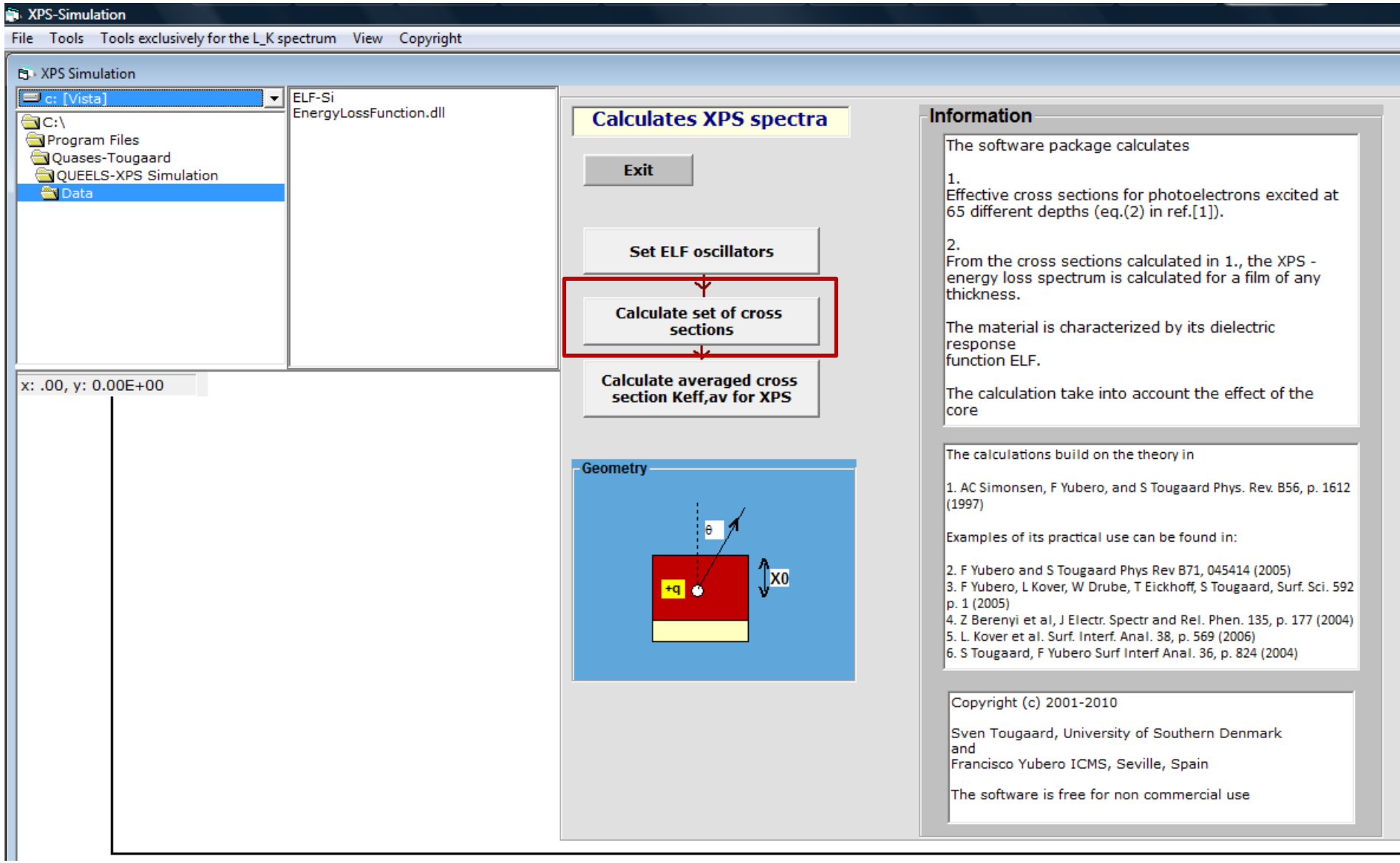
What is KK - sum rule

Plot ELF
E_Max = 100
E_step = 0.1
Plot ELF

x: 72.90, y: 2.962



$$\mathrm{Im}\left(-\frac{1}{\varepsilon(k,\omega)}\right)=\sum_i \frac{A_i\gamma_i\hbar\omega}{\left(\left(\hbar\omega_{0i}+\alpha_i\cdot\frac{\hbar^2k^2}{2m}\right)-\hbar^2\omega^2\right)^2+(\gamma_i\hbar\omega)^2}$$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c: [Vista]
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Program Files
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QUEELS-XPS Simulation
Data
ELF-Si
EnergyLossFunction.dll
x: .00, y: 0.00E+00
Calculates XPS spectra
Exit
Set ELF oscillators
Calculate set of cross sections
Calculate averaged cross section Keff,av for XPS
Geometry
θ
+q
X0
Information
The software package calculates
1.
Effective cross sections for photoelectrons excited at 65 different depths (eq.(2) in ref.[1]).
2.
From the cross sections calculated in 1., the XPS - energy loss spectrum is calculated for a film of any thickness.
The material is characterized by its dielectric response
function ELF.
The calculation take into account the effect of the core
The calculations build on the theory in
1. AC Simonsen, F Yubero, and S Tougaard Phys. Rev. B56, p. 1612 (1997)
Examples of its practical use can be found in:
2. F Yubero and S Tougaard Phys Rev B71, 045414 (2005)
3. F Yubero, L Kover, W Drube, T Eickhoff, S Tougaard, Surf. Sci. 592 p. 1 (2005)
4. Z Berenyi et al, J Electr. Spectr and Rel. Phen. 135, p. 177 (2004)
5. L. Kover et al. Surf. Interf. Anal. 38, p. 569 (2006)
6. S Tougaard, F Yubero Surf Interf Anal. 36, p. 824 (2004)
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Francisco Yubero ICMS, Seville, Spain
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C:\
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QUEELS-XPS Simulation
Data

ELF-Si
EnergyLossFunction.dll

Effective cross sections for photon excited electrons calculated for a wide

1. Click ELF data file in filelist

2. Press Read ELF file ELF-Si

3. Set these parameters

Ep = 1388 Emax = 30 Theta 0 n_integr: 250
Estep = 0.25 Emin = 1 q-hole = 1

4. Press button: Calculate Keff(X0)

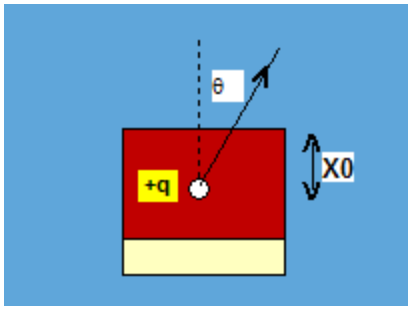
Data arrays are saved in these files (names can be changed)

Keff-total(X0)	Si2p-Keff-XPS-Total	Save for specific X0
Keff electr contrib.(X0)	Si2p-Keff-XPS-Electr	Save for specific X0
Keff hole contrib.(X0)	Si2p-Keff-XPS-hole	Save for specific X0

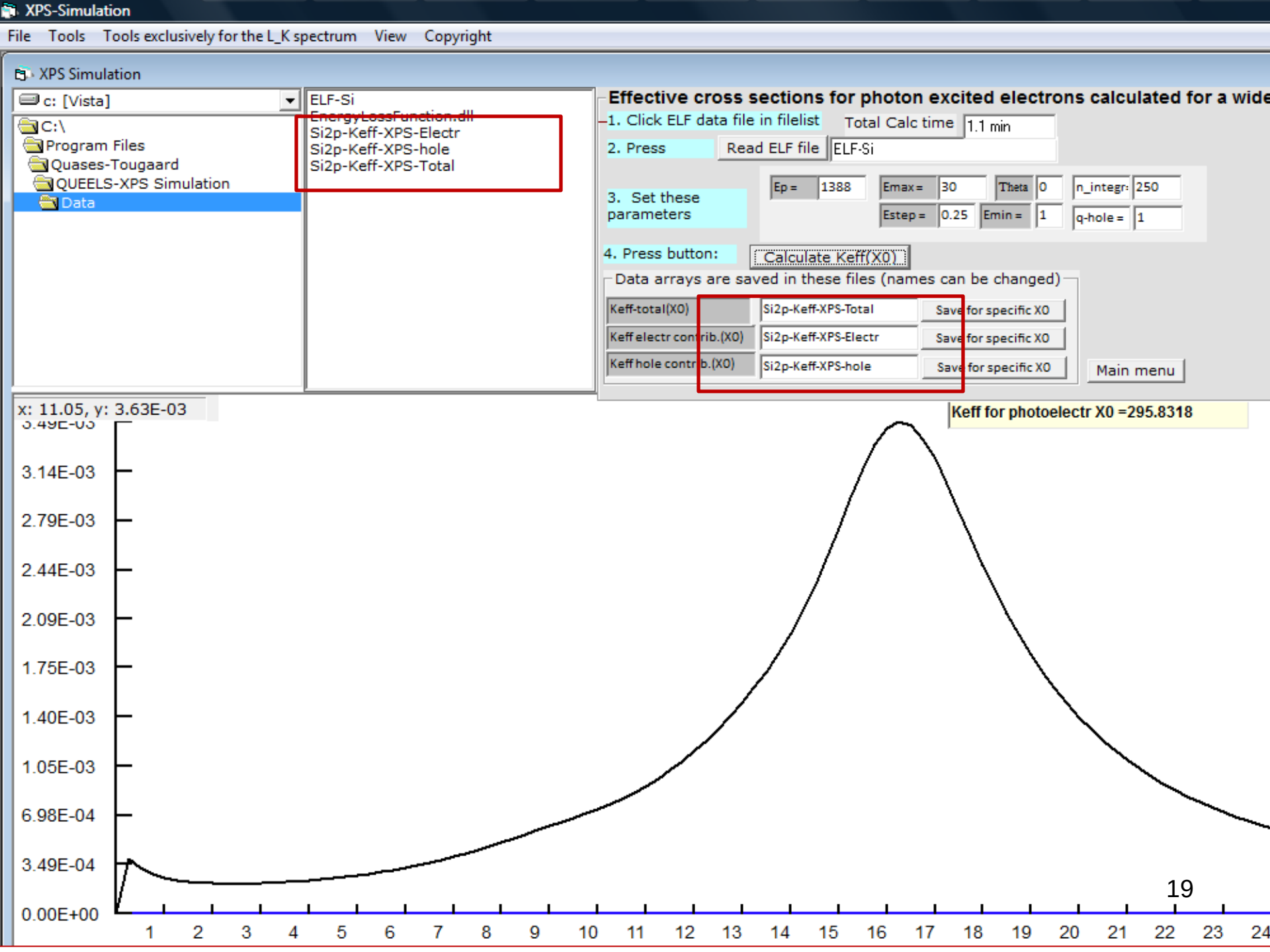
Main menu

x: 49.23, y: 1.76

ELF function: Im(-1/epsilon)



Calculates differential cross sections for 65 depths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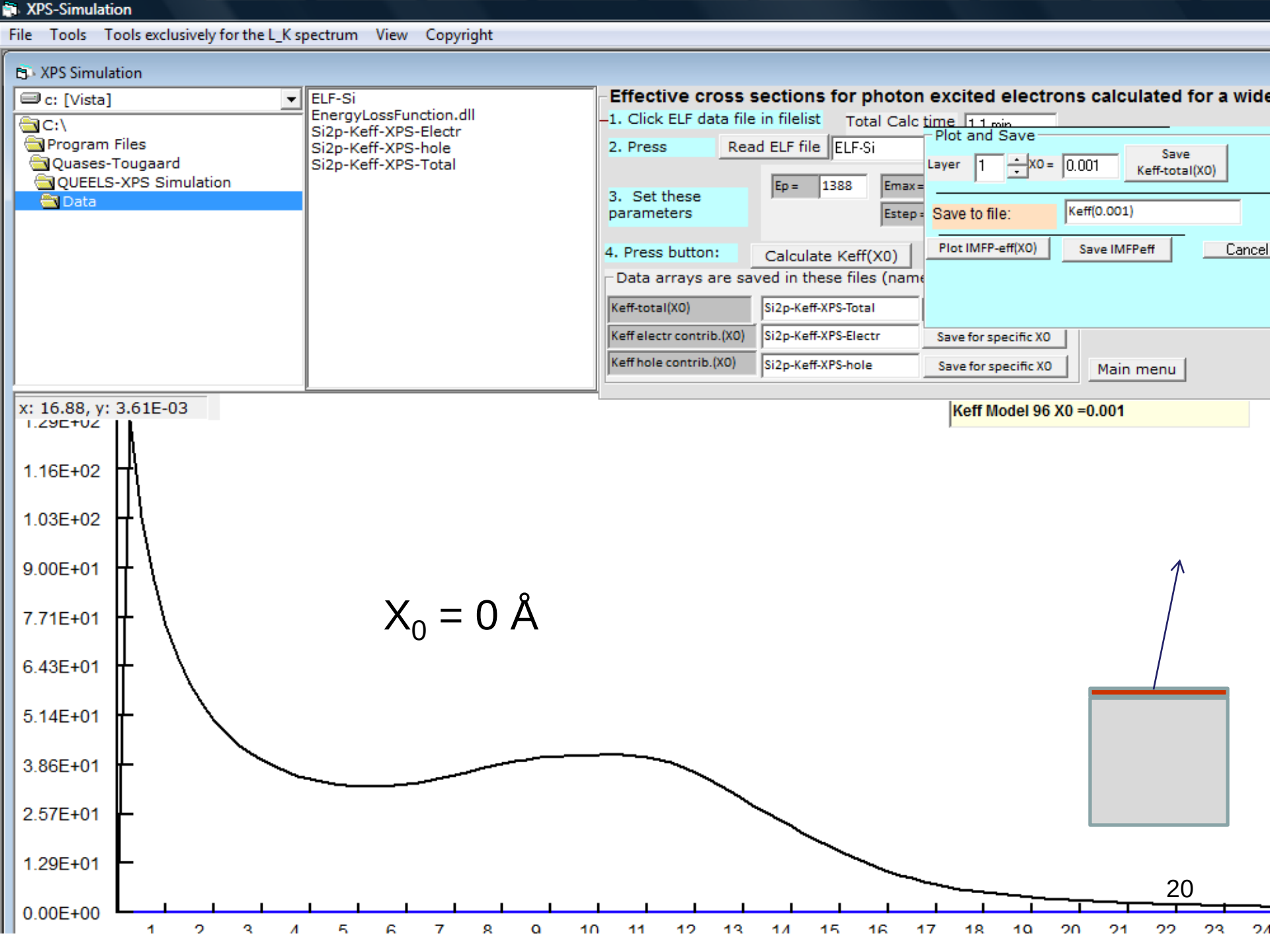
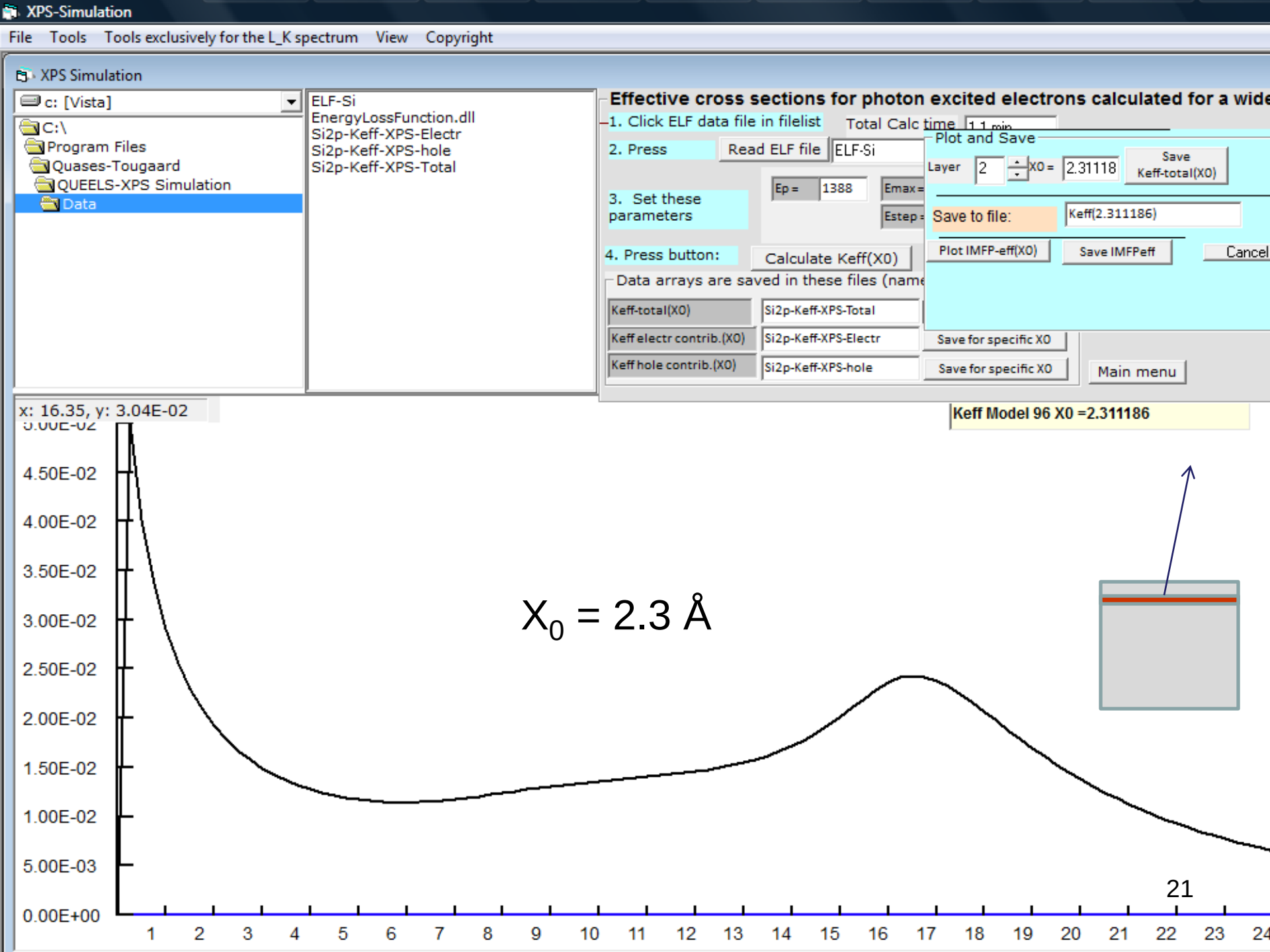
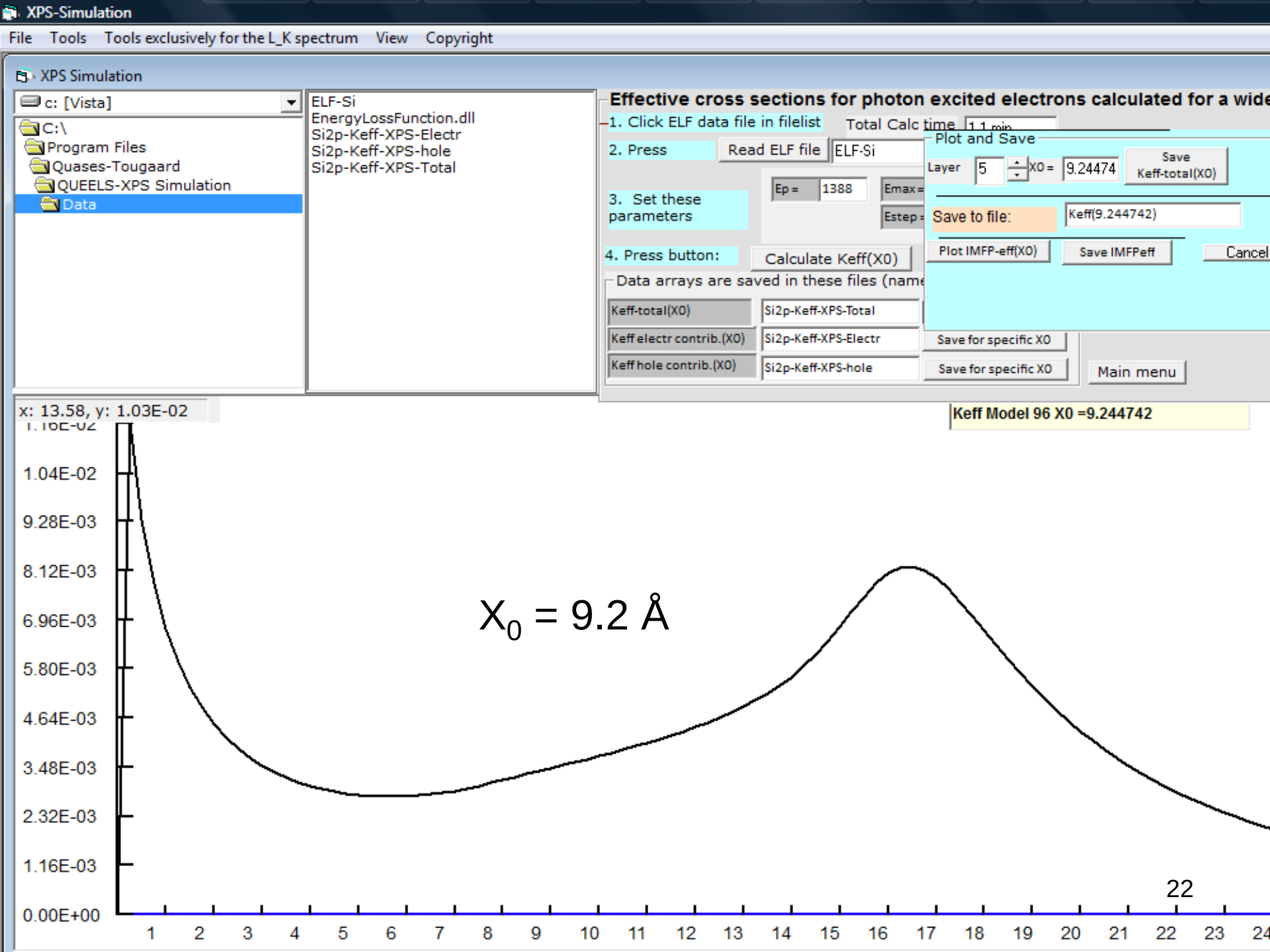
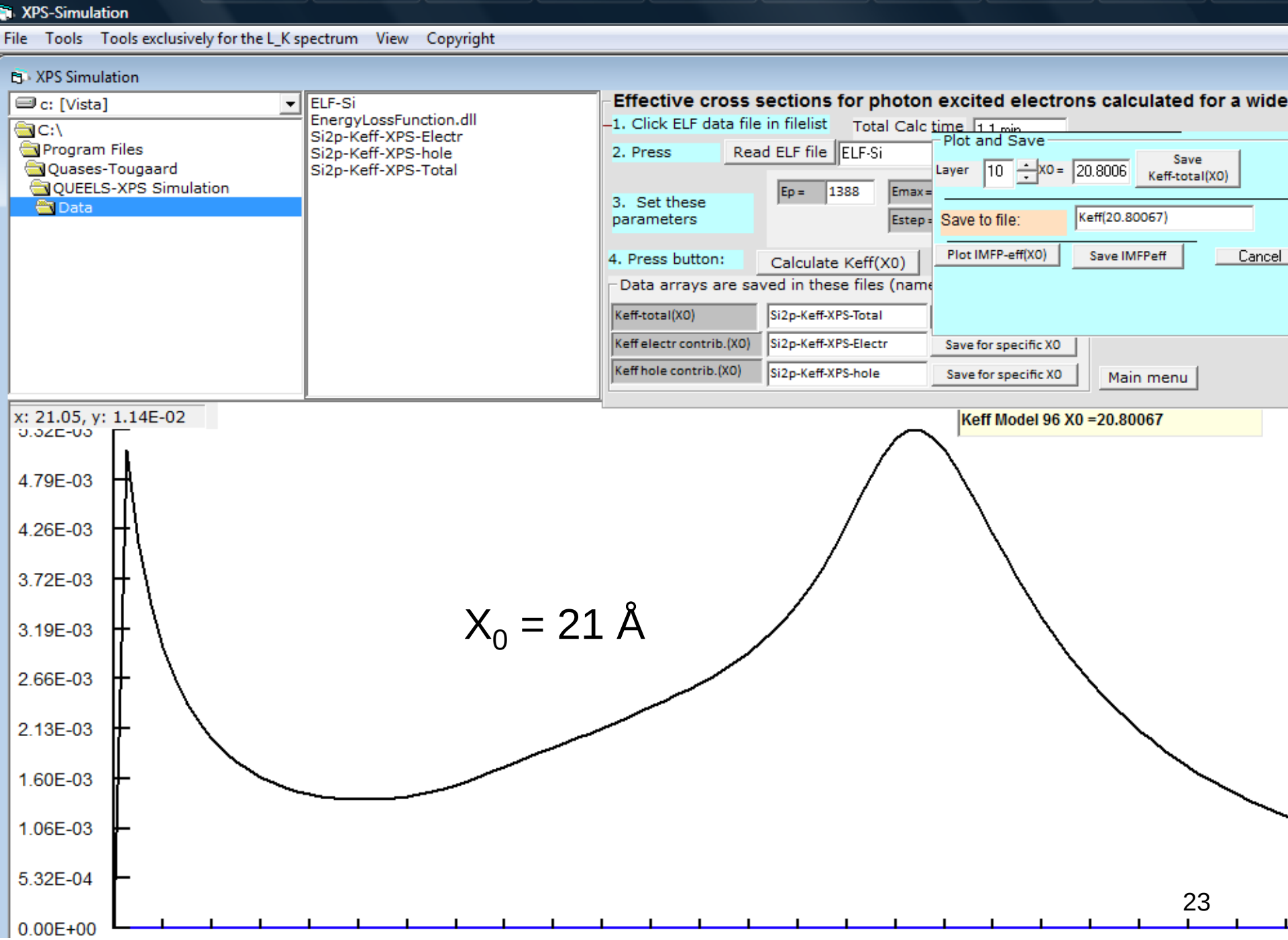
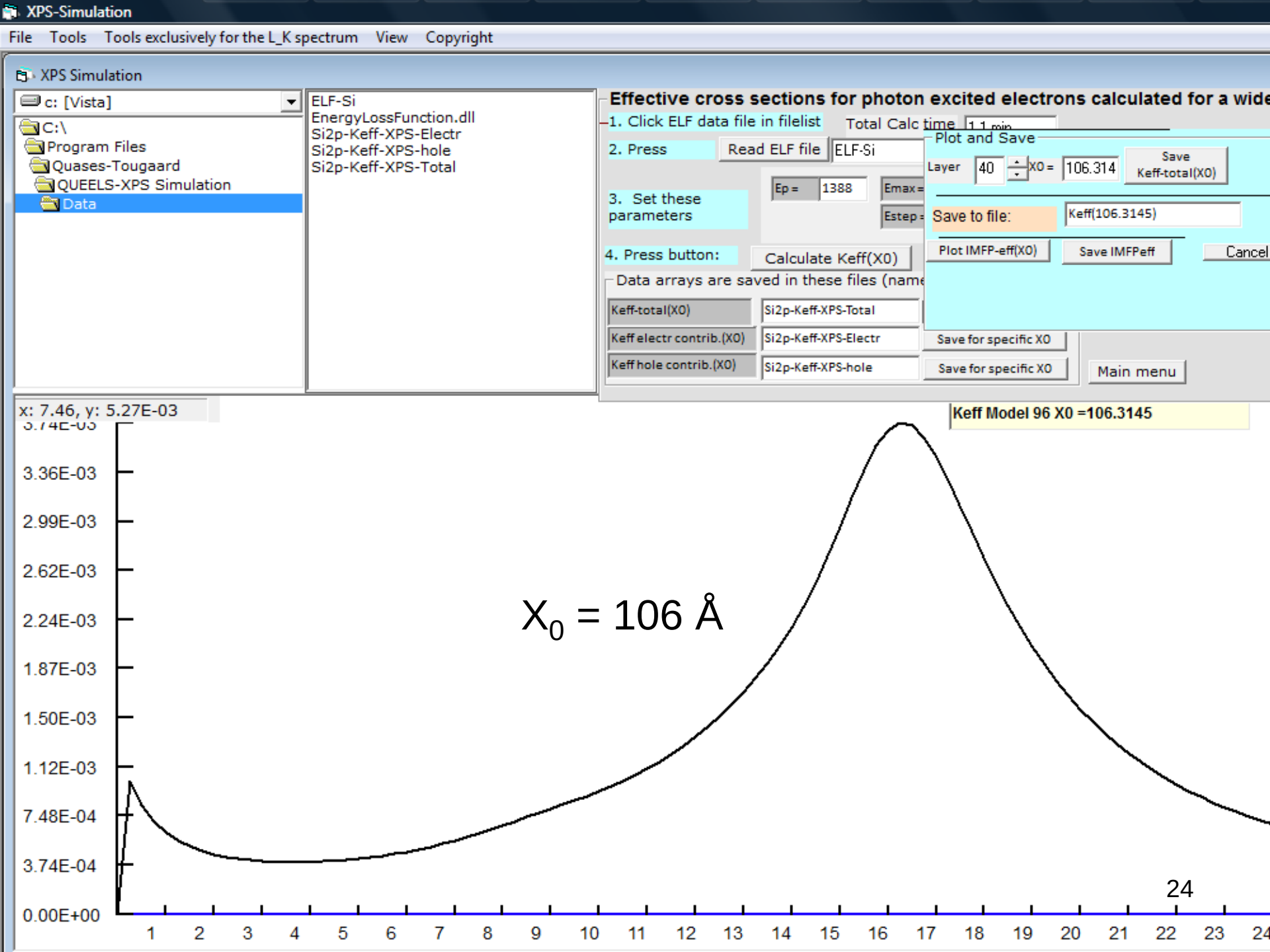
Data
ELF-Si
EnergyLossFunction.dll
Si2p-Keff-XPS-Electr
Si2p-Keff-XPS-hole
Si2p-Keff-XPS-Total
Effective cross sections for photon excited electrons calculated for a wide
1. Click ELF data file in filelist
Total Calc time
1.1 min
2. Press
Read ELF file
ELF-Si
3. Set these parameters
Ep =
1388
Emax =
30
Theta
0
n_integr:
250
Estep =
0.25
Emin =
1
q-hole =
1
4. Press button:
Calculate Keff(X0)
Data arrays are saved in these files (names can be changed)
Keff-total(X0)
Si2p-Keff-XPS-Total
Save for specific X0
Keff electr contrib.(X0)
Si2p-Keff-XPS-Electr
Save for specific X0
Keff hole contrib.(X0)
Si2p-Keff-XPS-hole
Save for specific X0
Main menu
x: 11.05, y: 3.63E-03
Keff for photoelectr X0 =295.8318
3.14E-03
2.79E-03
2.44E-03
2.09E-03
1.75E-03
1.40E-03
1.05E-03
6.98E-04
3.49E-04
0.00E+00
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24


XPS-Simulation
File Tools Tools exclusively for the L_K spectrum View Copyright
XPS Simulation
c: [Vista]
C:\
Program Files
Quases-Tougaard
QUEELS-XPS Simulation
Data
ELF-Si
EnergyLossFunction.dll
Si2p-Keff-XPS-Electr
Si2p-Keff-XPS-hole
Si2p-Keff-XPS-Total
Effective cross sections for photon excited electrons calculated for a wide
1. Click ELF data file in filelist
Total Calc time
2. Press
Read ELF file
ELF-Si
Plot and Save
Layer
1
X0 =
0.001
Save Keff-total(X0)
3. Set these parameters
Ep =
1388
Emax =
Estep =
Save to file:
Keff(0.001)
4. Press button:
Calculate Keff(X0)
Plot IMFP-eff(X0)
Save IMFPeff
Cancel
Data arrays are saved in these files (name
Keff-total(X0)
Si2p-Keff-XPS-Total
Keff electr contrib.(X0)
Si2p-Keff-XPS-Electr
Save for specific X0
Keff hole contrib.(X0)
Si2p-Keff-XPS-hole
Save for specific X0
Main menu
x: 16.88, y: 3.61E-03
Keff Model 96 X0 =0.001
1.16E+02
1.03E+02
9.00E+01
7.71E+01
6.43E+01
5.14E+01
3.86E+01
2.57E+01
1.29E+01
0.00E+00
X0 = 0 Å
20


XPS-Simulation
File Tools Tools exclusively for the L_K spectrum View Copyright
XPS Simulation
c: [Vista]
C:\
Program Files
Quases-Tougaard
QUEELS-XPS Simulation
Data
ELF-Si
EnergyLossFunction.dll
Si2p-Keff-XPS-Electr
Si2p-Keff-XPS-hole
Si2p-Keff-XPS-Total
Effective cross sections for photon excited electrons calculated for a wide
1. Click ELF data file in filelist
Total Calc time
2. Press
Read ELF file
ELF-Si
Plot and Save
Layer
2
X0 =
2.31118
Save Keff-total(X0)
3. Set these parameters
Ep =
1388
Emax =
Estep =
Save to file:
Keff(2.311186)
4. Press button:
Calculate Keff(X0)
Plot IMFP-eff(X0)
Save IMFPeff
Cancel
Data arrays are saved in these files (name
Keff-total(X0)
Si2p-Keff-XPS-Total
Keff electr contrib.(X0)
Si2p-Keff-XPS-Electr
Save for specific X0
Keff hole contrib.(X0)
Si2p-Keff-XPS-hole
Save for specific X0
Main menu
x: 16.35, y: 3.04E-02
Keff Model 96 X0 =2.311186
4.50E-02
4.00E-02
3.50E-02
3.00E-02
2.50E-02
2.00E-02
1.50E-02
1.00E-02
5.00E-03
0.00E+00
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
X_0 = 2.3 Å
21


XPS-Simulation
File Tools Tools exclusively for the L_K spectrum View Copyright
XPS Simulation
c: [Vista]
C:\
Program Files
Quases-Tougaard
QUEELS-XPS Simulation
Data
ELF-Si
EnergyLossFunction.dll
Si2p-Keff-XPS-Electr
Si2p-Keff-XPS-hole
Si2p-Keff-XPS-Total
Effective cross sections for photon excited electrons calculated for a wide
1. Click ELF data file in filelist
Total Calc time
2. Press
Read ELF file
ELF-Si
Plot and Save
Layer
5
X0 =
9.24474
Save Keff-total(X0)
3. Set these parameters
Ep =
1388
Emax =
Estep =
Save to file:
Keff(9.244742)
4. Press button:
Calculate Keff(X0)
Plot IMFP-eff(X0)
Save IMFPeff
Cancel
Data arrays are saved in these files (name
Keff-total(X0)
Si2p-Keff-XPS-Total
Keff electr contrib.(X0)
Si2p-Keff-XPS-Electr
Save for specific X0
Keff hole contrib.(X0)
Si2p-Keff-XPS-hole
Save for specific X0
Main menu
x: 13.58, y: 1.03E-02
Keff Model 96 X0 =9.244742
1.04E-02
9.28E-03
8.12E-03
6.96E-03
5.80E-03
4.64E-03
3.48E-03
2.32E-03
1.16E-03
0.00E+00
X0 = 9.2 Å
22
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24


XPS-Simulation
File Tools Tools exclusively for the L_K spectrum View Copyright
XPS Simulation
c: [Vista]
C:\
Program Files
Quases-Tougaard
QUEELS-XPS Simulation
Data
ELF-Si
EnergyLossFunction.dll
Si2p-Keff-XPS-Electr
Si2p-Keff-XPS-hole
Si2p-Keff-XPS-Total
Effective cross sections for photon excited electrons calculated for a wide
1. Click ELF data file in filelist
Total Calc time
2. Press
Read ELF file
ELF-Si
Plot and Save
Layer
10
X0 =
20.8006
Save Keff-total(X0)
3. Set these parameters
Ep =
1388
Emax =
Estep =
Save to file:
Keff(20.80067)
4. Press button:
Calculate Keff(X0)
Plot IMFP-eff(X0)
Save IMFPeff
Cancel
Data arrays are saved in these files (name
Keff-total(X0)
Si2p-Keff-XPS-Total
Keff electr contrib.(X0)
Si2p-Keff-XPS-Electr
Save for specific X0
Keff hole contrib.(X0)
Si2p-Keff-XPS-hole
Save for specific X0
Main menu
x: 21.05, y: 1.14E-02
Keff Model 96 X0 =20.80067
4.79E-03
4.26E-03
3.72E-03
3.19E-03
2.66E-03
2.13E-03
1.60E-03
1.06E-03
5.32E-04
0.00E+00
X0 = 21 Å
23


XPS-Simulation
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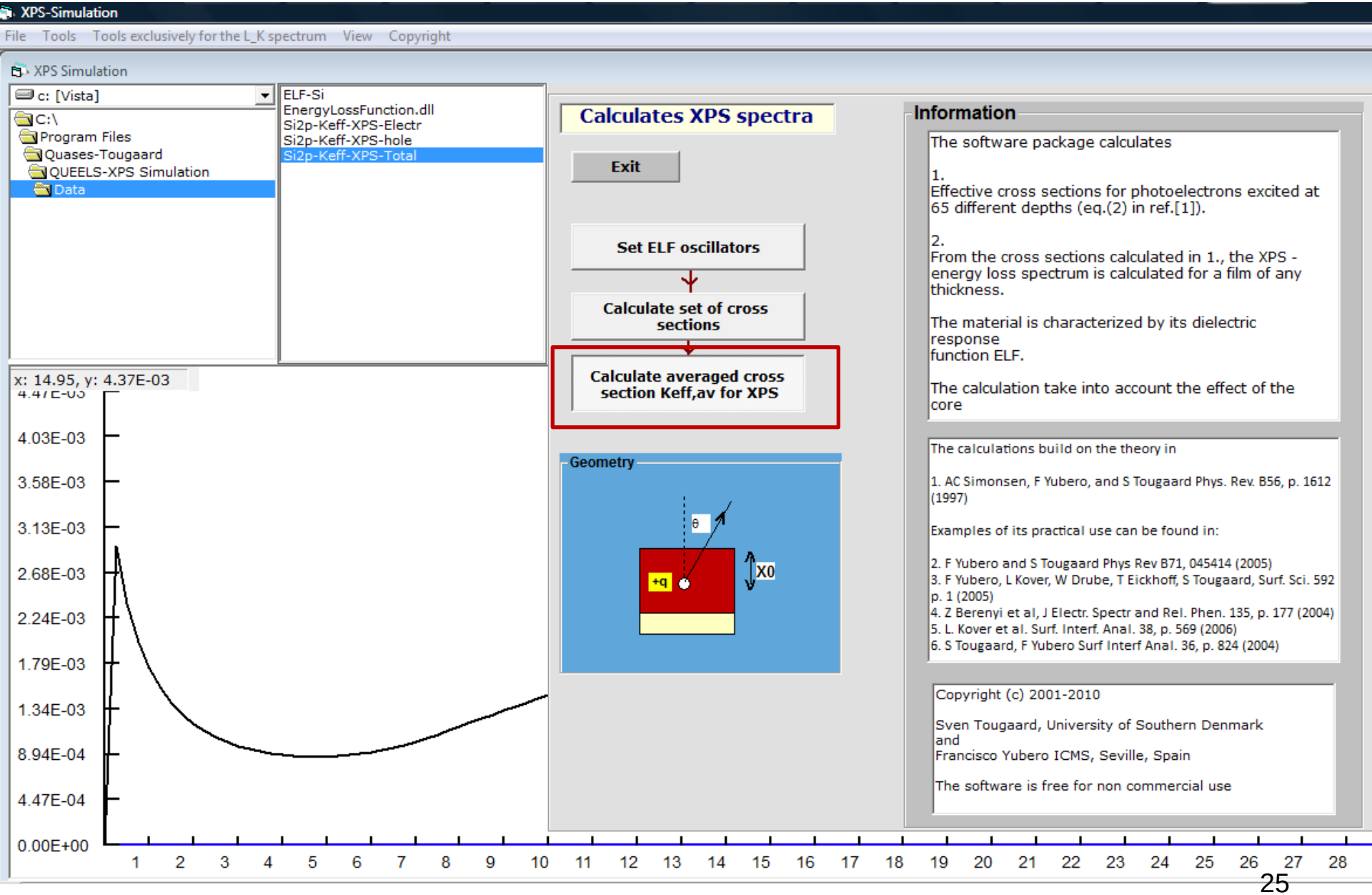
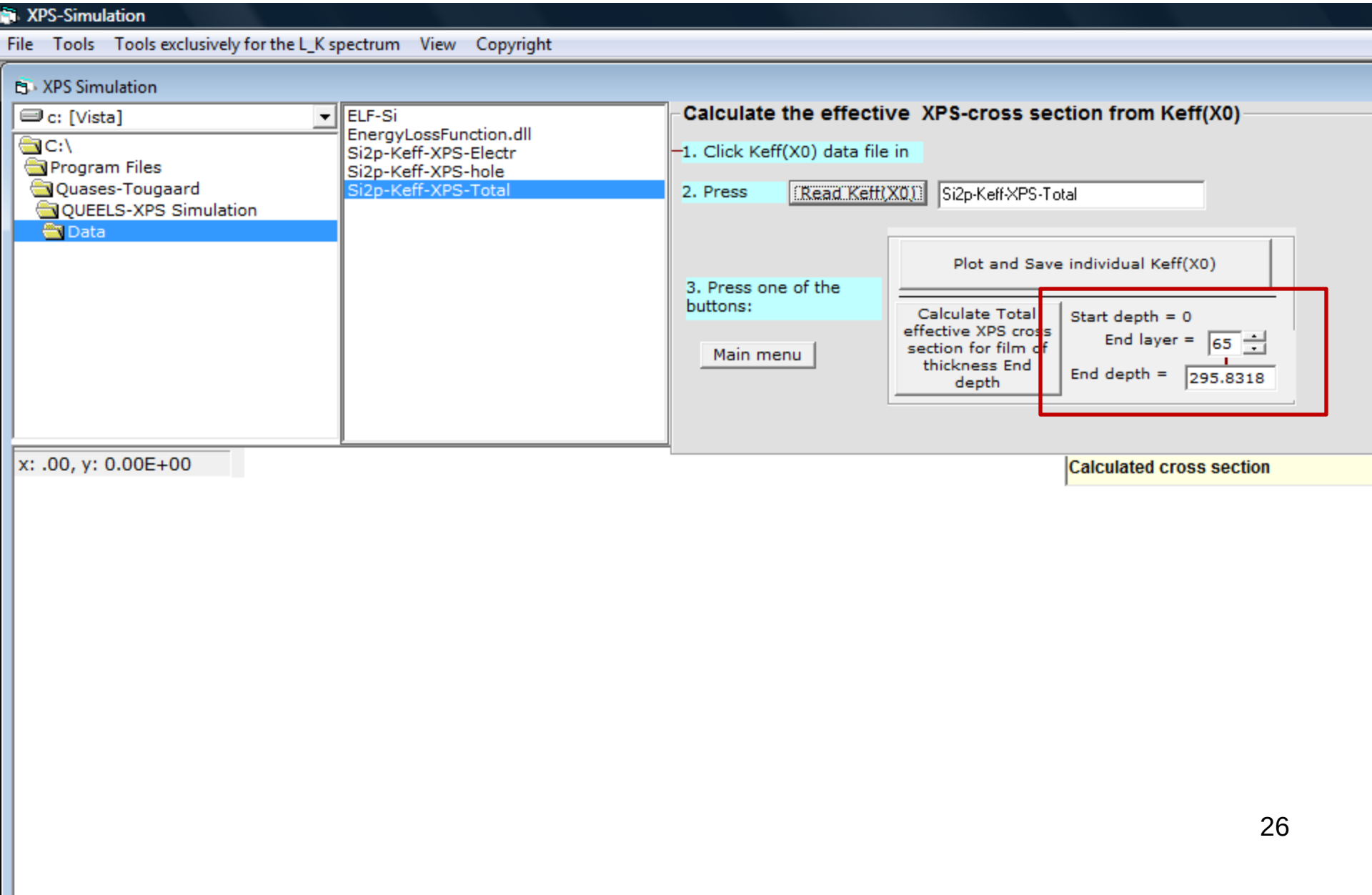
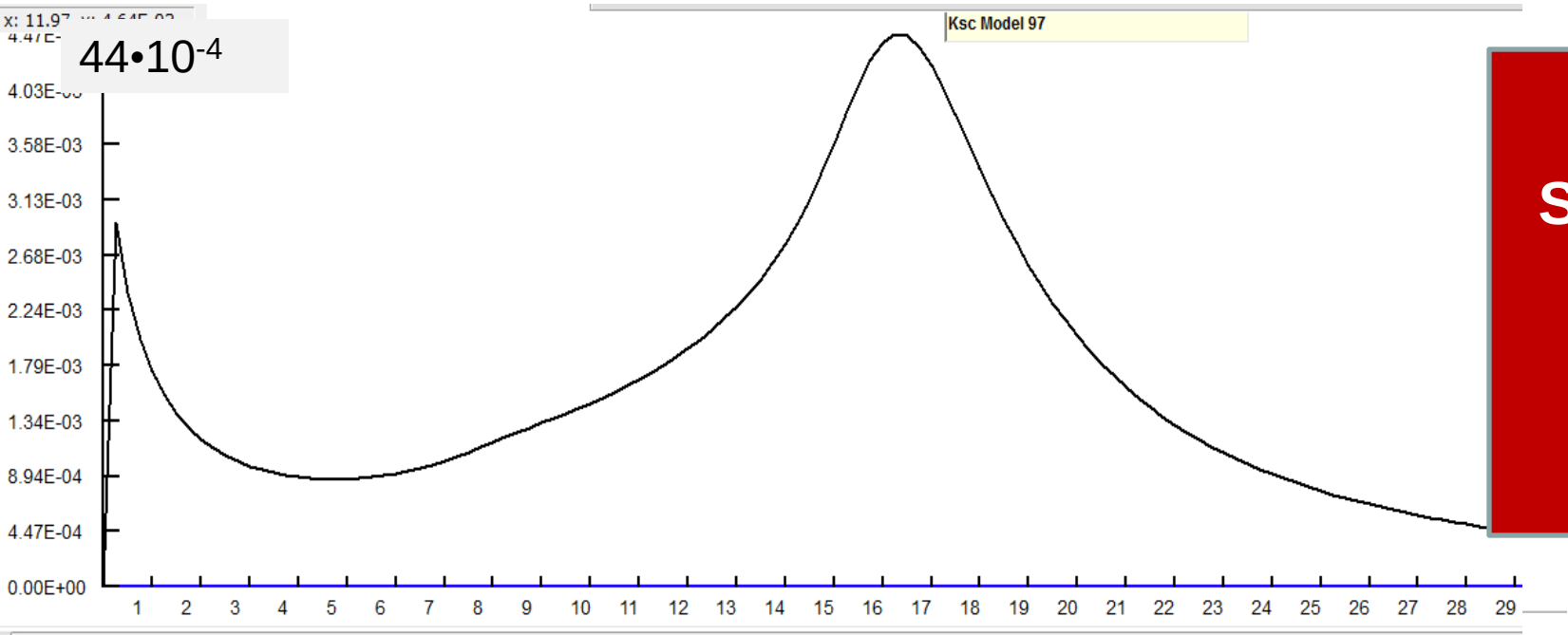
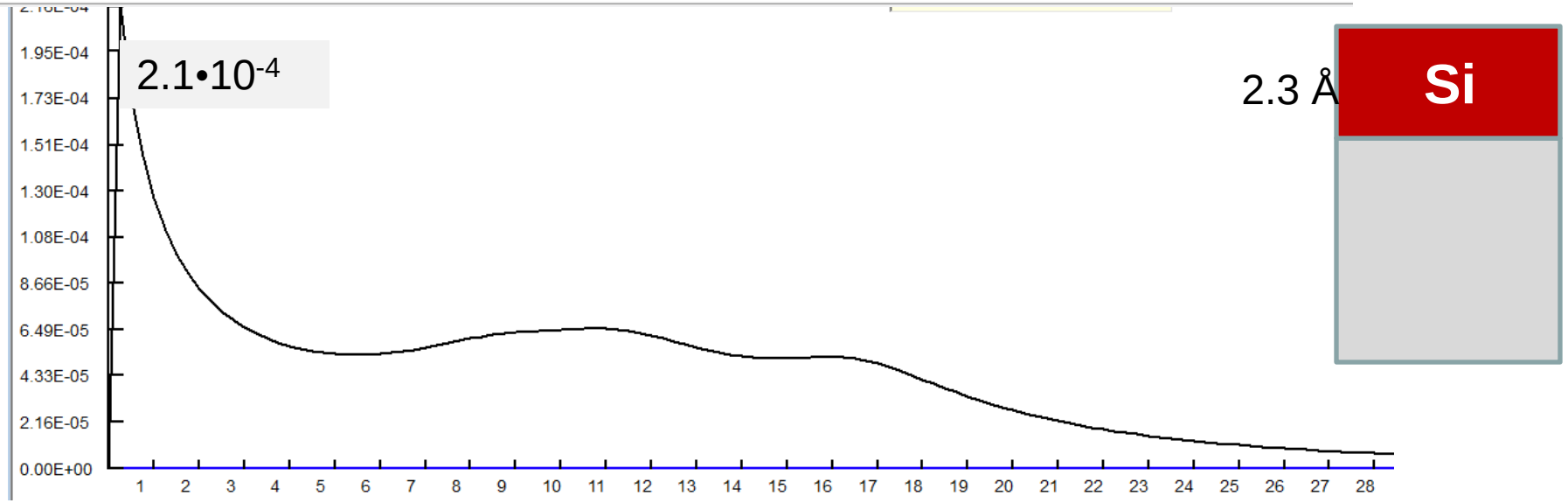
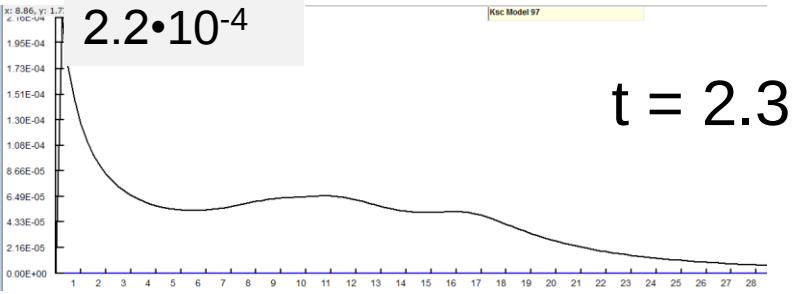
XPS Simulation
c: [Vista]
C:\
Program Files
Quases-Tougaard
QUEELS-XPS Simulation
Data
ELF-Si
EnergyLossFunction.dll
Si2p-Keff-XPS-Electr
Si2p-Keff-XPS-hole
Si2p-Keff-XPS-Total
Effective cross sections for photon excited electrons calculated for a wide
1. Click ELF data file in filelist
Total Calc time
2. Press
Read ELF file
ELF-Si
Plot and Save
Layer
40
X0 =
106.314
Save Keff-total(X0)
3. Set these parameters
Ep =
1388
Emax =
Estep =
Save to file:
Keff(106.3145)
4. Press button:
Calculate Keff(X0)
Plot IMFP-eff(X0)
Save IMFPeff
Cancel
Data arrays are saved in these files (name
Keff-total(X0)
Si2p-Keff-XPS-Total
Keff electr contrib.(X0)
Si2p-Keff-XPS-Electr
Save for specific X0
Keff hole contrib.(X0)
Si2p-Keff-XPS-hole
Save for specific X0
Main menu
x: 7.46, y: 5.27E-03
Keff Model 96 X0 =106.3145
3.36E-03
2.99E-03
2.62E-03
2.24E-03
1.87E-03
1.50E-03
1.12E-03
7.48E-04
3.74E-04
0.00E+00
X0 = 106 Å
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
24


XPS-Simulation
File Tools Tools exclusively for the L_K spectrum View Copyright
XPS Simulation
c: [Vista]
C:\
Program Files
Quases-Tougaard
QUEELS-XPS Simulation
Data
ELF-Si
EnergyLossFunction.dll
Si2p-Keff-XPS-Electr
Si2p-Keff-XPS-hole
Si2p-Keff-XPS-Total
Calculates XPS spectra
Exit
Set ELF oscillators
Calculate set of cross sections
Calculate averaged cross section Keff,av for XPS
Geometry
θ
+q
X0
Information
The software package calculates
1.
Effective cross sections for photoelectrons excited at 65 different depths (eq.(2) in ref.[1]).
2.
From the cross sections calculated in 1., the XPS - energy loss spectrum is calculated for a film of any thickness.
The material is characterized by its dielectric response
function ELF.
The calculation take into account the effect of the core
The calculations build on the theory in
1. AC Simonsen, F Yubero, and S Tougaard Phys. Rev. B56, p. 1612 (1997)
Examples of its practical use can be found in:
2. F Yubero and S Tougaard Phys Rev B71, 045414 (2005)
3. F Yubero, L Kover, W Drube, T Eickhoff, S Tougaard, Surf. Sci. 592 p. 1 (2005)
4. Z Berenyi et al, J Electr. Spectr and Rel. Phen. 135, p. 177 (2004)
5. L. Kover et al. Surf. Interf. Anal. 38, p. 569 (2006)
6. S Tougaard, F Yubero Surf Interf Anal. 36, p. 824 (2004)
Copyright (c) 2001-2010
Sven Tougaard, University of Southern Denmark
and
Francisco Yubero ICMS, Seville, Spain
The software is free for non commercial use
x: 14.95, y: 4.37E-03
4.03E-03
3.58E-03
3.13E-03
2.68E-03
2.24E-03
1.79E-03
1.34E-03
8.94E-04
4.47E-04
0.00E+00
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28


XPS-Simulation
File
Tools
Tools exclusively for the L_K spectrum
View
Copyright
XPS Simulation
c: [Vista]
C:\
Program Files
Quases-Tougaard
QUEELS-XPS Simulation
Data
ELF-Si
EnergyLossFunction.dll
Si2p-Keff-XPS-Electr
Si2p-Keff-XPS-hole
Si2p-Keff-XPS-Total
Calculate the effective XPS-cross section from Keff(X0)
1. Click Keff(X0) data file in
2. Press
Read Keff(X0)
Si2p-Keff-XPS-Total
Plot and Save individual Keff(X0)
3. Press one of the buttons:
Calculate Total effective XPS cross section for film of thickness End depth
Start depth = 0
End layer =
65
End depth =
295.8318
Main menu
x: .00, y: 0.00E+00
Calculated cross section

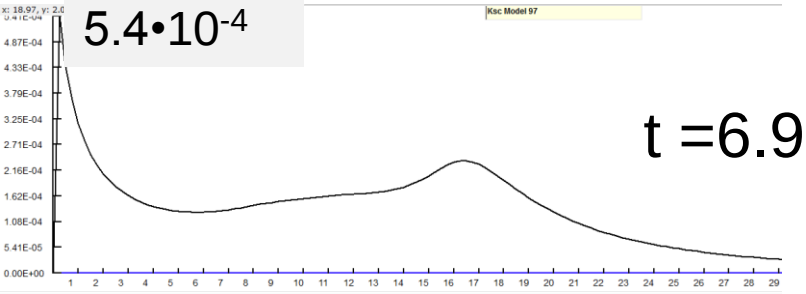

Ksc Model 97
44•10-4
4.03E-03
3.58E-03
3.13E-03
2.68E-03
2.24E-03
1.79E-03
1.34E-03
8.94E-04
4.47E-04
0.00E+00
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29
Si

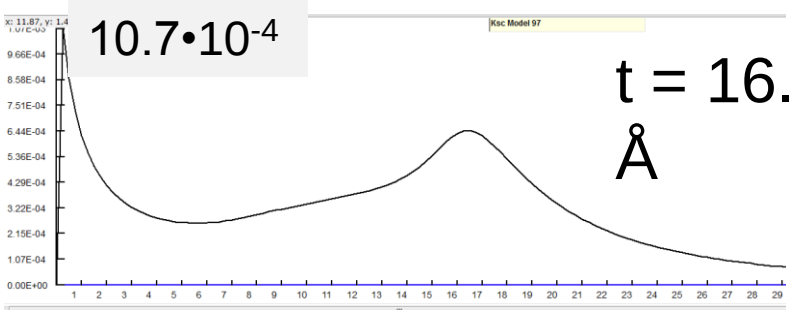

2.1•10-4
1.95E-04
1.73E-04
1.51E-04
1.30E-04
1.08E-04
8.66E-05
6.49E-05
4.33E-05
2.16E-05
0.00E+00
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28
2.3 Å
Si

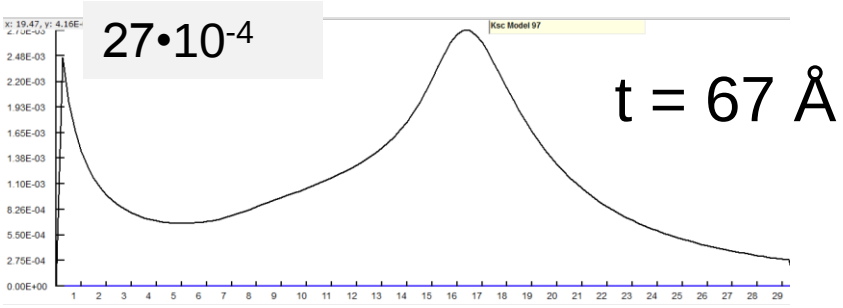

2.2•10-4
t = 2.3 Å

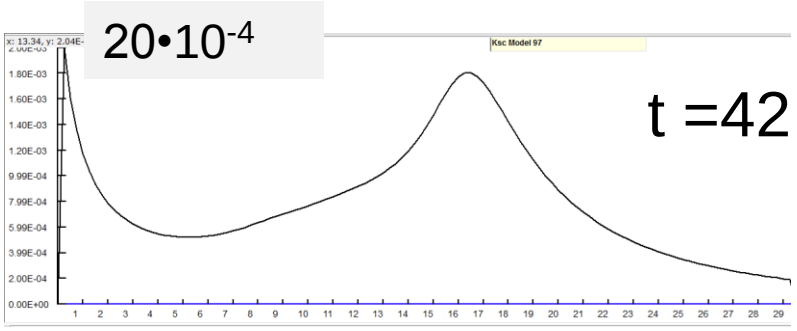
t

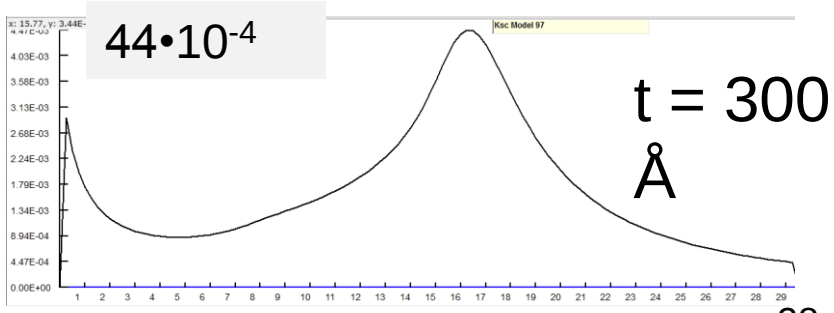
Si


5.4•10-4
t =6.9 Å


10.7•10-4
t = 16.2 Å


27•10-4
t = 67 Å


20•10-4
t =42 Å


44•10-4
t = 300 Å

QUEELS-XPS software package
Semi-classical dielectric response model

1. QUEELS-ε(k,ω)-REELS Semi-classical dielectric response model

2. The XPS- Semiclassical dielectric response model

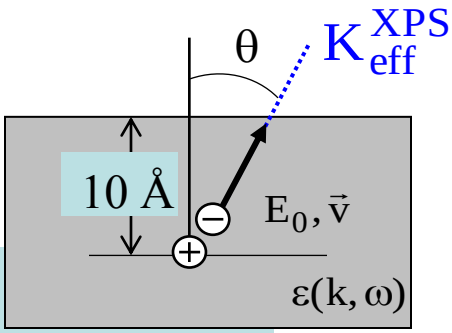
   Extrinsic and intrinsic excitations

3. The QUEELS-XPS software Package

4. The validity of the model

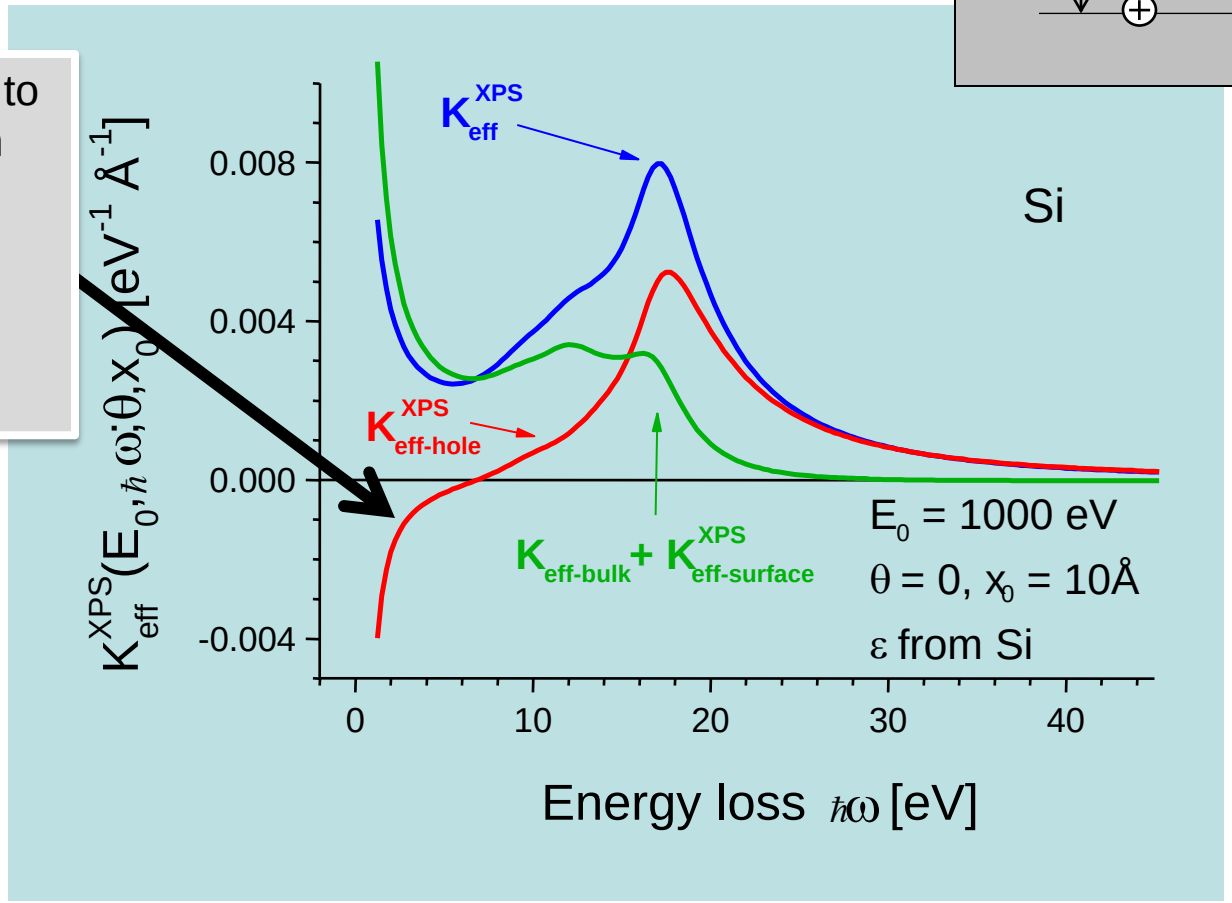
   quantitative comparison with experiments

Effect of the static hole



The negative part is due to the interference between surface, core, and bulk excitations.

The total cross sect is always > 0.



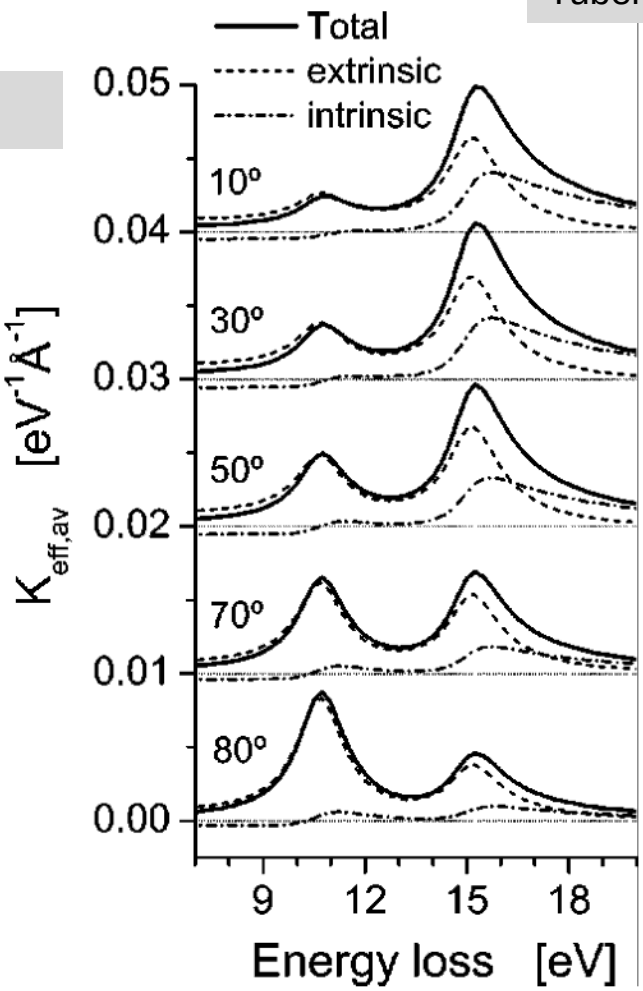
The hole contributes with a significant intensity to the bulk plasmon

ST,FY: SIA 36(2004)824

Effect of the static hole – intrinsic excitations

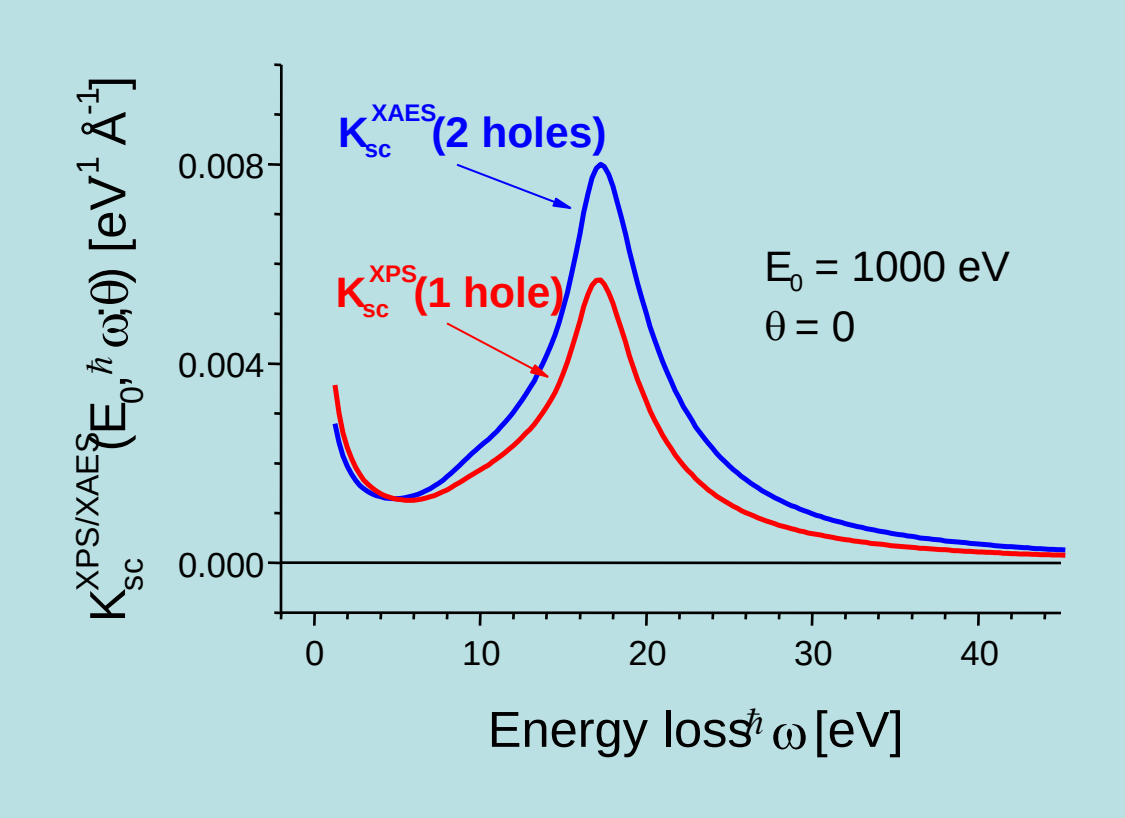
Yubero, Tougaard: SIA 36(2004)824

XPS- energy loss for Al



the hole contributes little to the surface plasmon but a lot to the bulk plasmon.

Two holes left behind… Auger emission



The intensity of the plasmon excited is larger for 2 holes than for 1 hole

Note: Only input in the theory is the dielectric function ε(k,ω)

ε(k,ω) can be taken

from litterature or

easily be determined from analysis of a REELS spectrum using the QUEELS-ε(k,ω)-REELS software package

QUEELS-XPS software package
Semi-classical dielectric response model

1. Intro: REELS Semi-classical dielectric response model
   QUEELS-ε(k,ω)-REELS software package

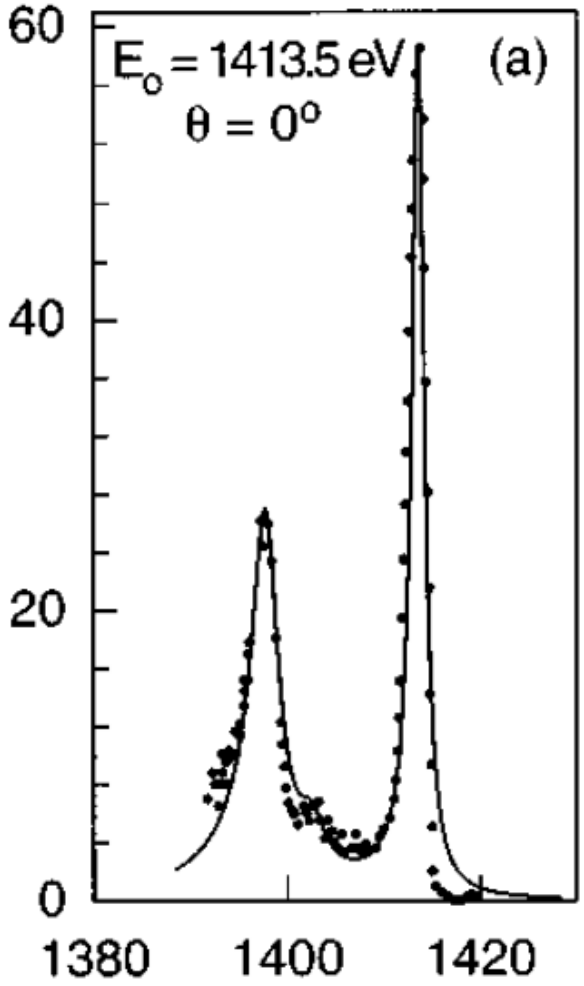
2. The XPS- Semiclassical dielectric response model
   Extrinsic and intrinsic excitations

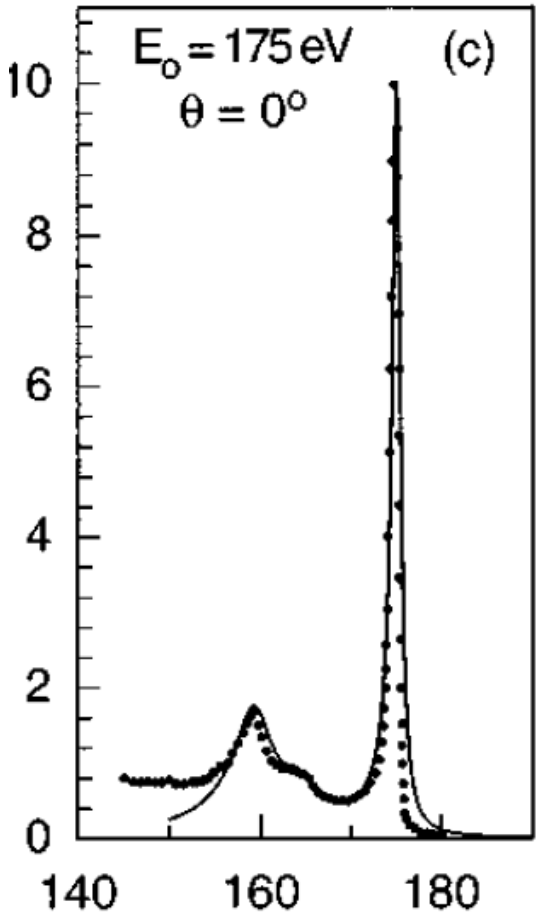
3. The QUEELS-XPS software Package

4. The validity of the model
   quantitative comparison with experiments

Si2p photoemission
compared to experiment

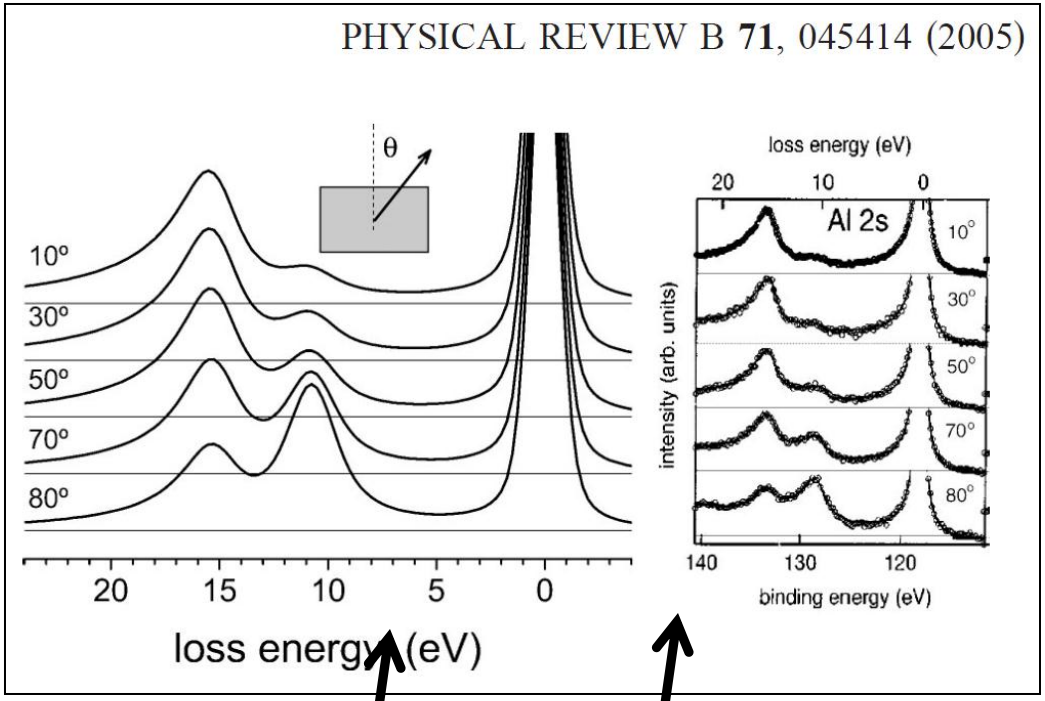
Phys. Rev.B56 (1997)1612





Variation of emission angle

Al 2s



XPS theory

XPS experiment

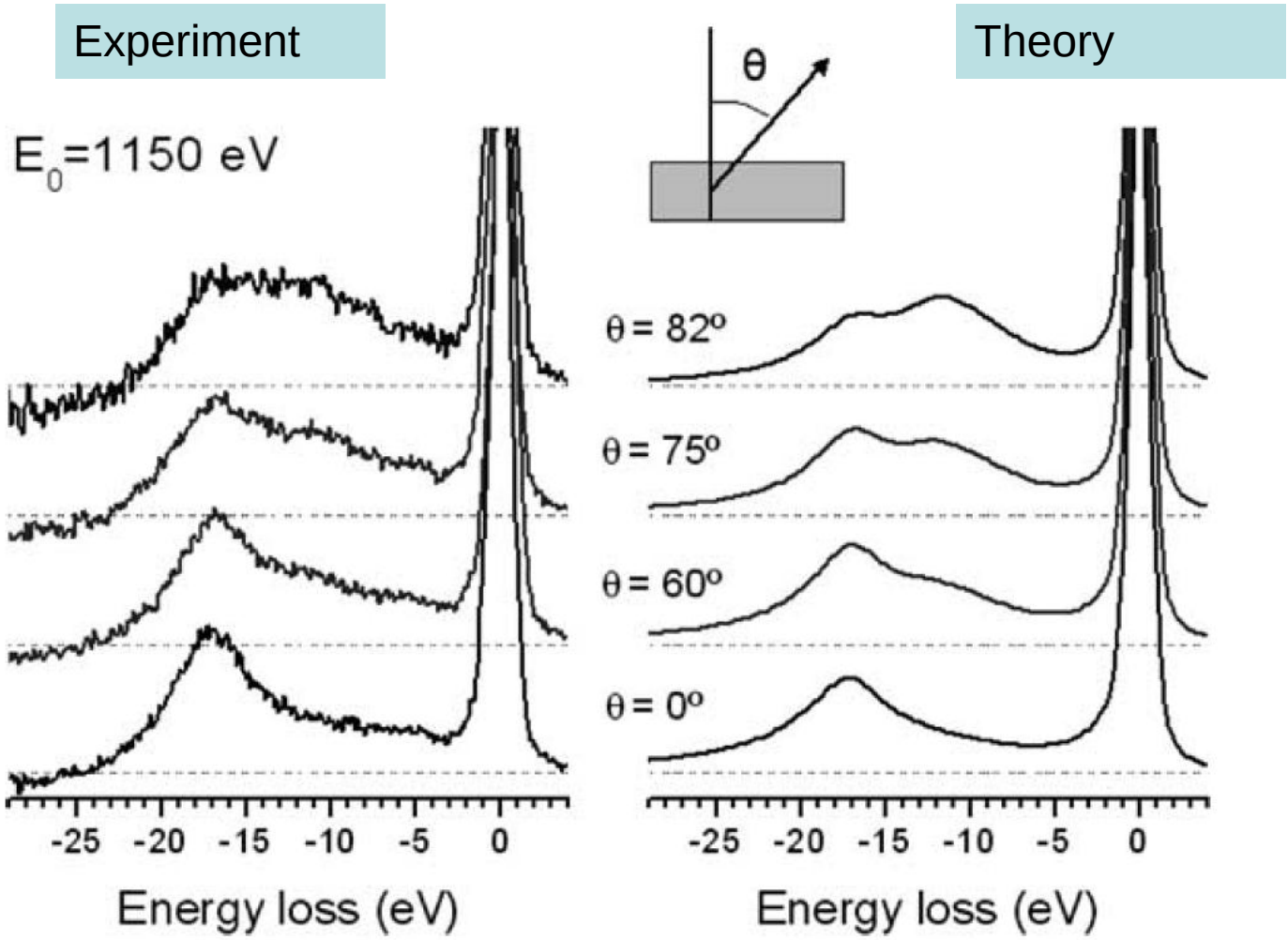
Comparison is on an absolute scale

Only input in the theory is ε(k,ω)

Variation of emission angle

Yubeo et al Surf Sci 592 (2005) 1

Si 2p



Variation of photon energy 225-850 eV

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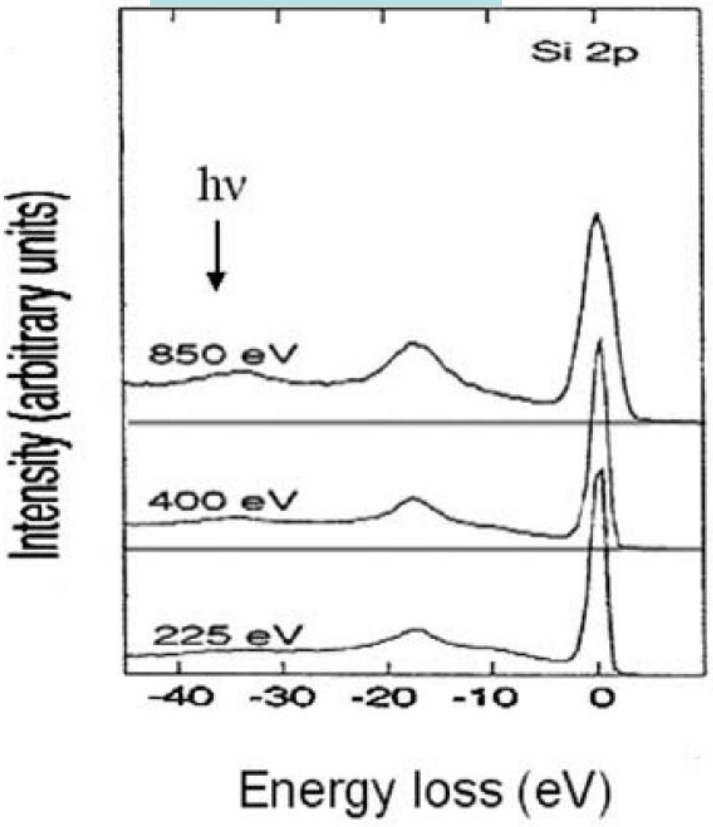
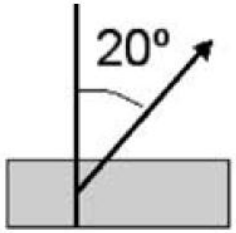
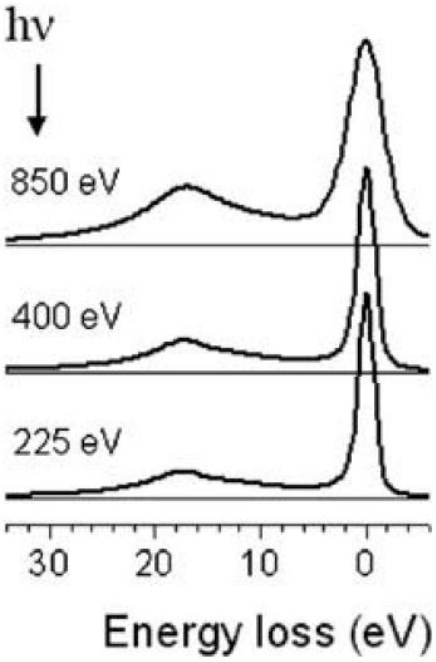
Experiment





Theory

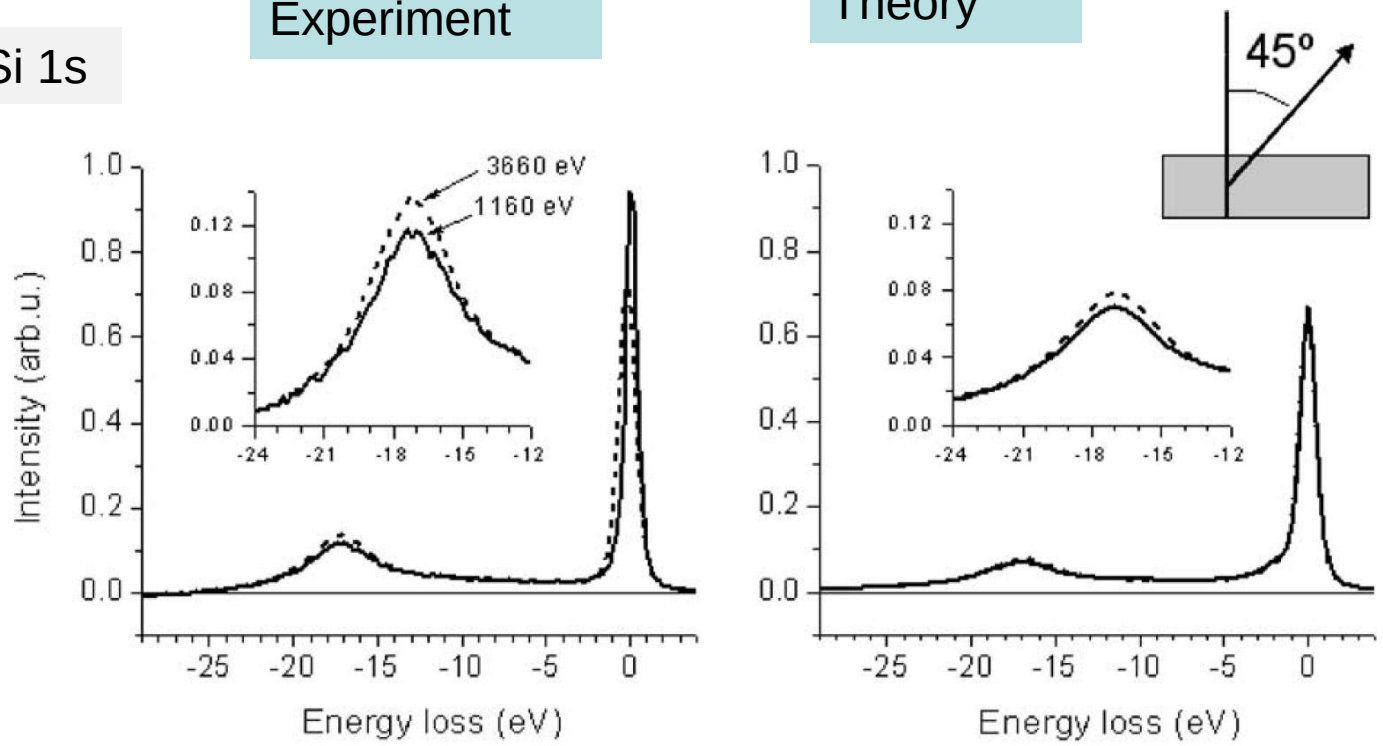


Variation of photon energy 3000 eV – 5500 eV

Si 1s

Experiment

Theory



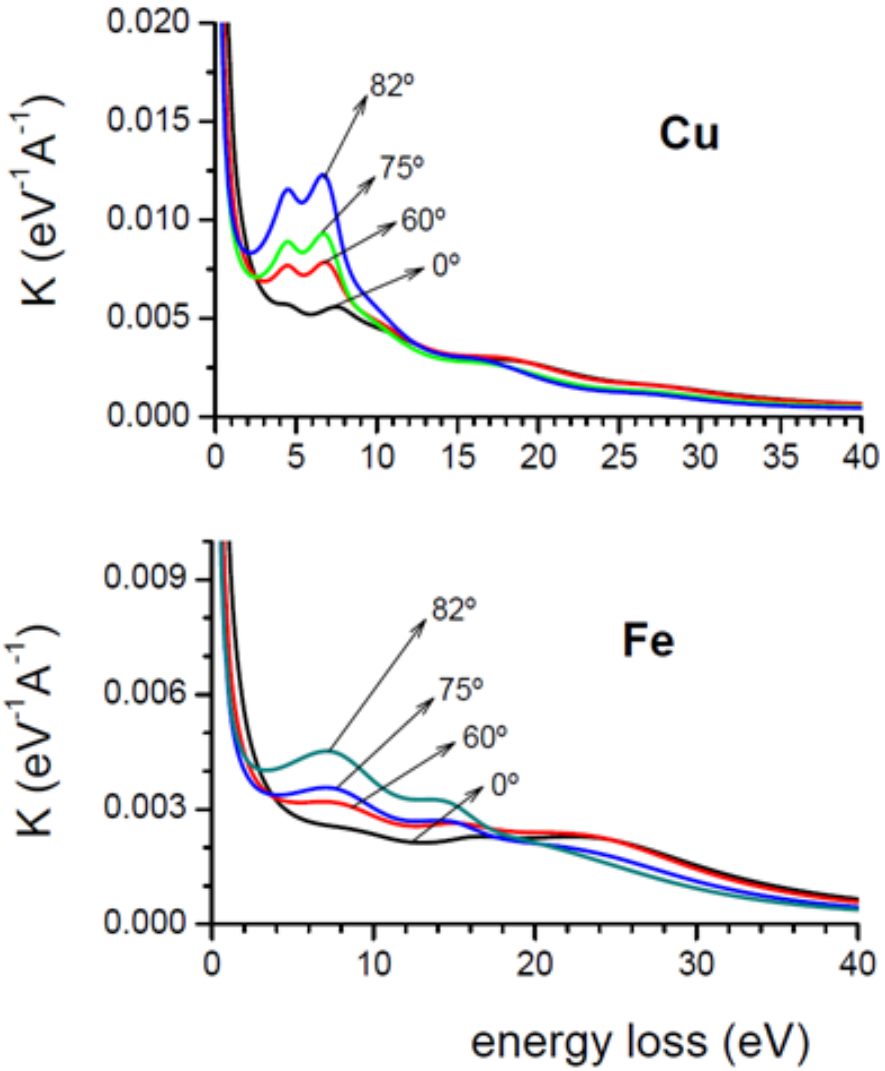
Higher photon energy gives larger intrinsic plasmon (less time to relax and screen the hole potential).

Transition metals Cu and Fe

F. Yubero and S. Tougaard to be publ.

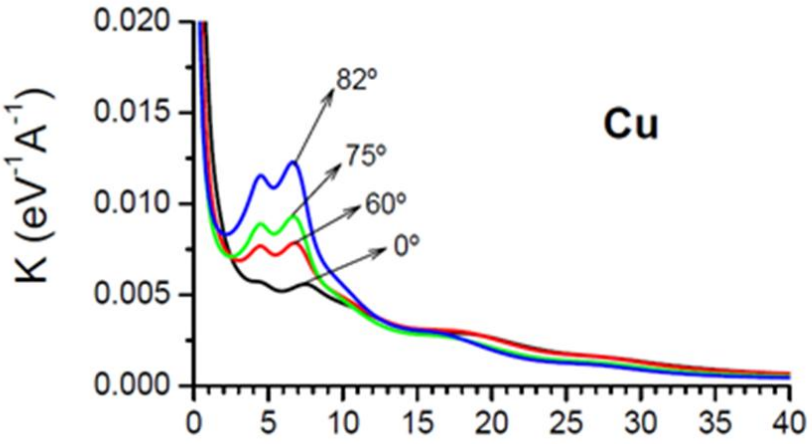
Theory

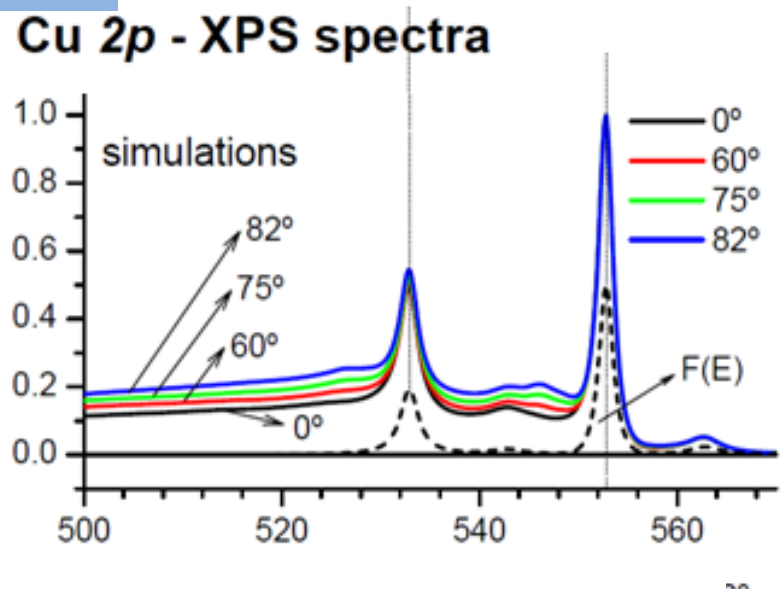
Calculated effective energy loss function K(T)



Theory

Effective energy loss function K(T)





$$J(E) \propto F(E) + \lambda \int_{E}^{\infty} F(E')K(E_0, E' - E)dE' + \sum_{n=2}^{\infty} J_n$$

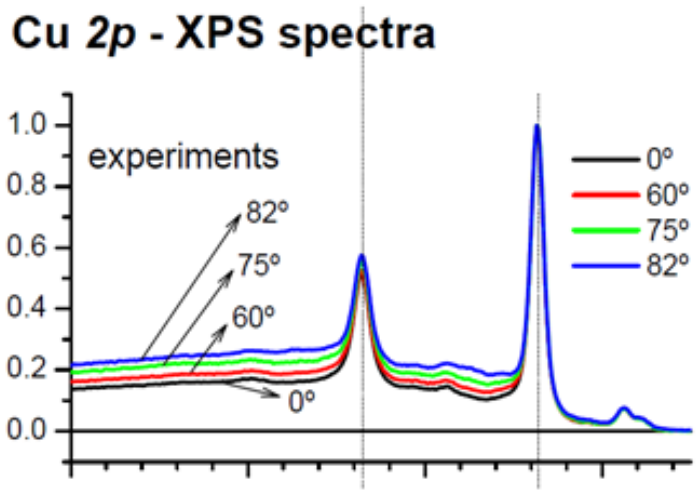
Photo-excited spectrum

First scattering

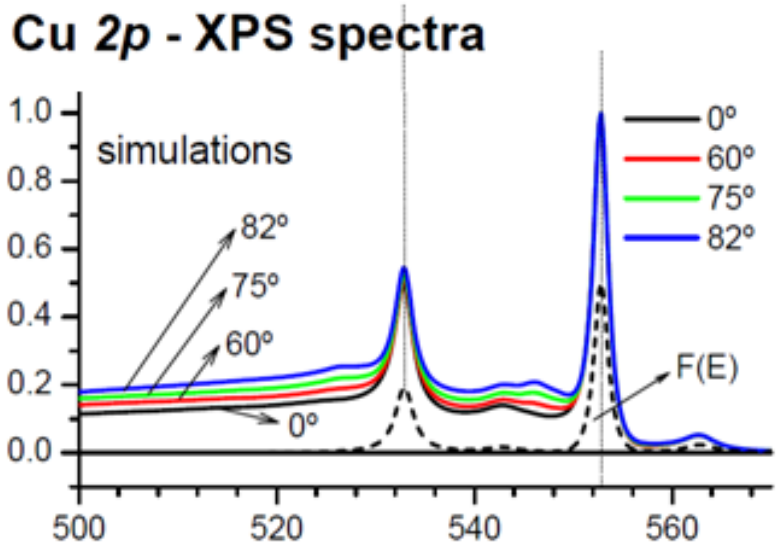
Multiple scattered electrons

Cu2p

Experiment



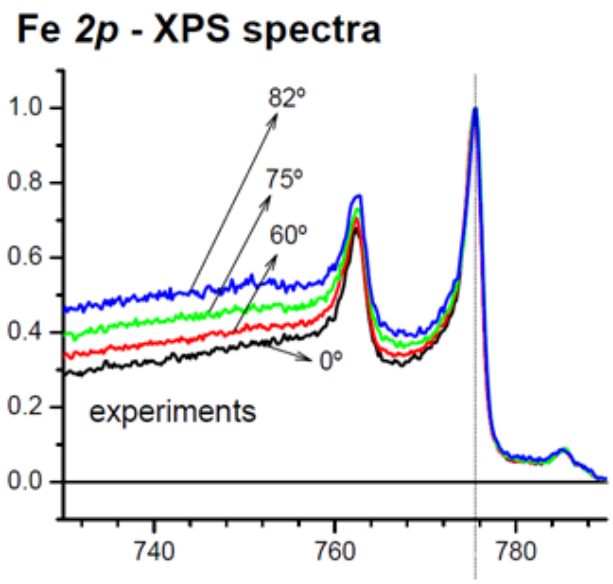
Theory

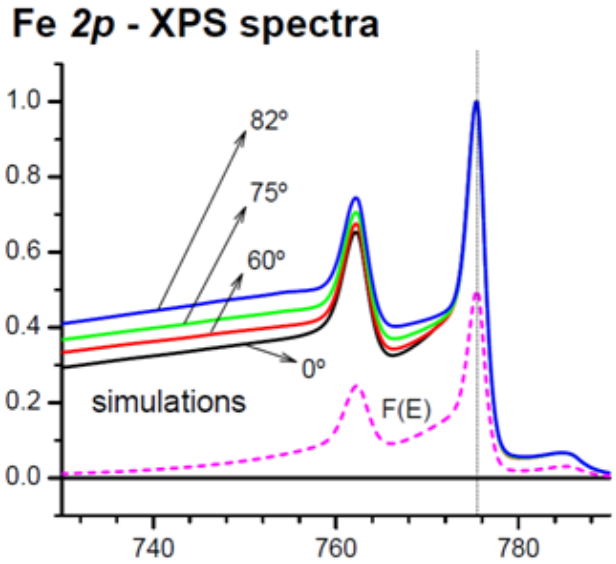


Experiment

Fe2p

Theory





QUEELS-XPS software package

Conclusion:

The semiclassical dielectric model for photoemission reproduces rather well quantitatively the angular and energy dependence of the energy loss processes

We hope the XPS-model and QUEELS-XPS software package will be useful to gain better quantitative understanding of the photo-excitation process

The software was used for the work presented by N. Pauly this morning

QUEELS-XPS software package
Semi-classical dielectric response model

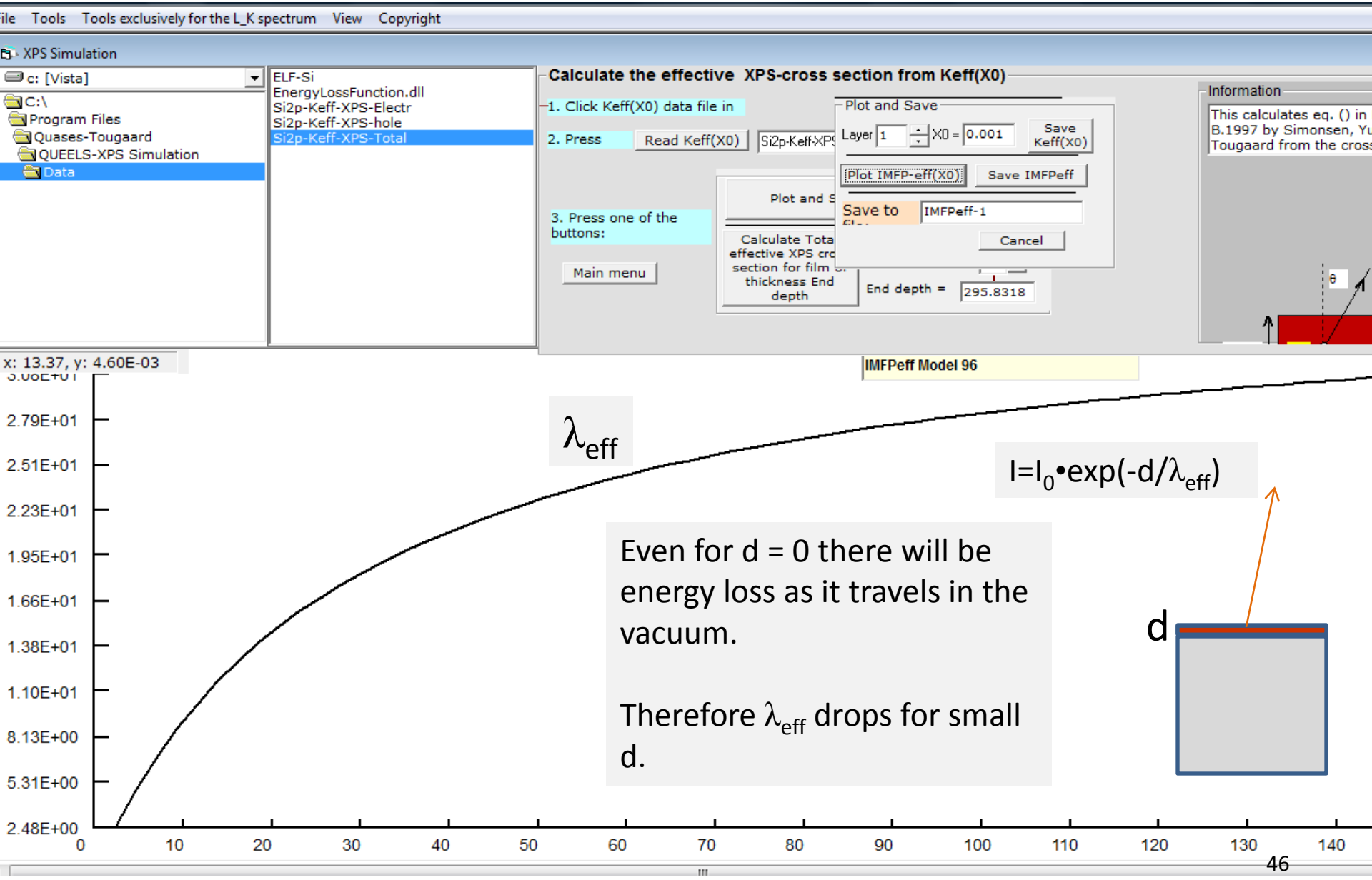
1. Intro: REELS Semi-classical dielectric response model
   QUEELS-ε(k,ω)-REELS software package

2. The XPS- Semiclassical dielectric response model
   Extrinsic and intrinsic excitations

3. The QUEELS-XPS software Package

4. The validity of the model
   quantitative comparison with experiments

The software was used in the talk by Nicolas Pauly Tuesday morning.
”New parameter to correct for surface and core hole effects in XPS”



λ_{eff}

$I=I_0 \bullet \exp(-d/\lambda_{eff})$

Even for d = 0 there will be energy loss as it travels in the vacuum.

Therefore λ_{eff} drops for small d.

d