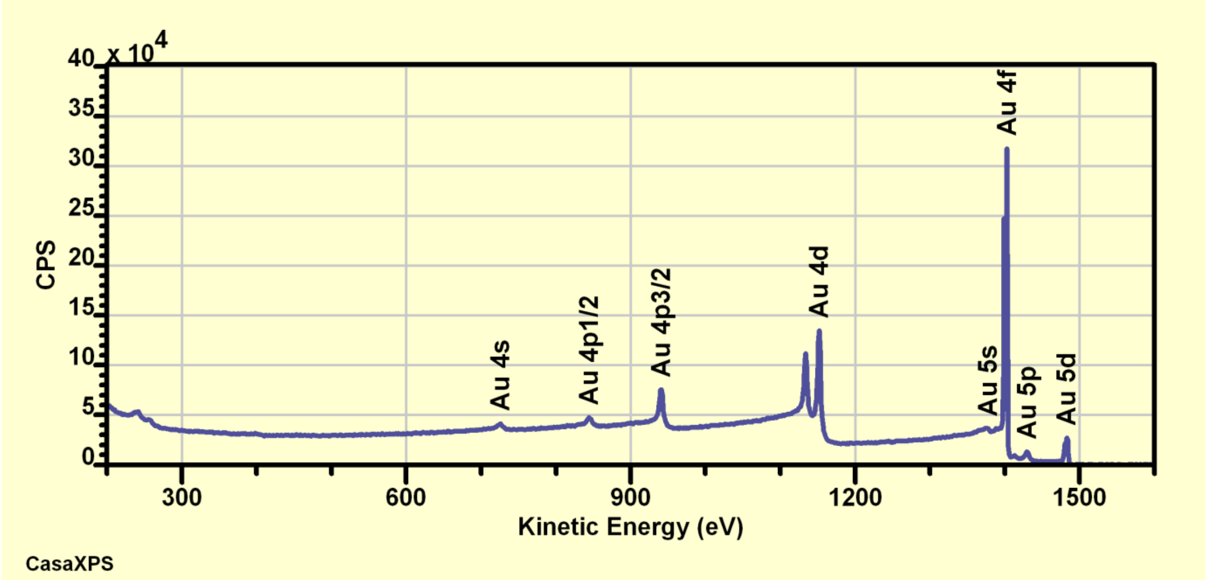
Quantification of Homogenous Samples

The following statement is intended to summarise the essence of quantification by XPS.

An atomic concentration computed from a XPS spectrum involves isolating emission peaks, one per element (XPS data in general include multiple emission peaks for each element), then performing a sequence of corrections to these spectral intensities leading to values (normalised peak intensities) representative of the amount of substance sampled by an XPS measurement.

Relative Sensitivity Factors



Essentially, the probability of a scattering of a photon by an atom leaving the final electronic configuration with a hole in a specific core electronic shell is dependent on which core level is altered in the final state. The relative intensities for these photoemission peaks depends on these probabilities for the final state configuration and therefore the number of electrons detected are not uniformly distributed between the set of photoemission peaks in an XPS spectrum from a given element, but appear as a sequence of emission peaks with varying intensity.

The purpose of Relative Sensitivity Factors (RSF) is to correct peak intensities to account for differences resulting from the photoemission process.

Theoretical RSF, referred to as Scofield cross-sections, are used to correct for peak intensity differences due to the photoemission process.

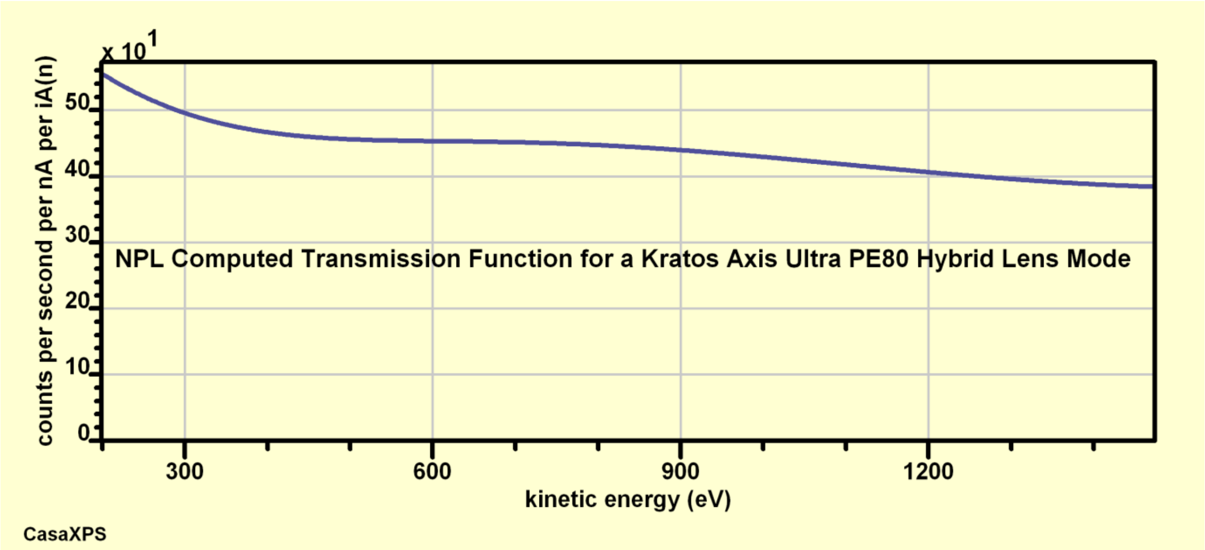
Transition probabilities calculated using Hartree-Slater approximations are tabulated by Scofield for photons of energy corresponding to Al and Mg x-ray sources. Scofield cross-sections do not account for angular distribution variation in the effective cross-section as a consequence of instruments detecting electrons in a specific direction relative to the photon source. Angular distribution correction to these Scofield cross-sections based on a given instrument geometry are applied resulting in RSF values appropriate for a given x-ray source and the angle between the x-ray source and the direction defined by the electron energy analyser.

Scofield cross-sections are corrected for angular distribution using the factor $1 - \frac{\beta}{4}(3\cos^2\theta - 1)$ relative to s-orbital electron configurations. The β value is computed for the element for which the Scofield cross-section is defined, and θ is the x-ray source to electron analyser angle. For data from a Kratos Axis Ultra the angle between the x-ray source and the direction of the electron analyser is assumed to be 60°. For an Ulvac PHI VersaProbe the angle θ is 45°. Magic angle instruments do not require angular distribution correction since the angle θ is chosen such that $3\cos^2\theta - 1 = 0$.

Instrumental Transmission Correction

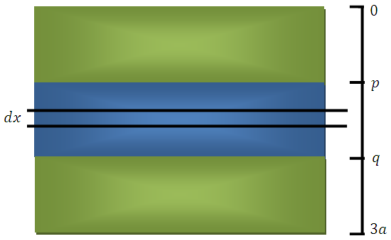
The number of electrons recorded by an instrument at a specific kinetic energy for the detected electrons deviate from the number of electrons emitted from the sample. The ratio of electrons leaving the sample to the number of electrons recorded at the detector varies as a function of the kinetic energy for the emitted electrons. To adjust for these variations in collection efficiency an instrument transmission function is measured.

Data in these examples are corrected for transmission using the National Physical Laboratory (NPL) transmission correction software. A transmission function is prepared for each operating mode for a given instrument. Differences in operating mode may include specific settings for the pass energy, electron optical lens modes, aperture settings and detector settings.



Escape Depth Correction

Inelastic scattering of electrons within solid state materials as measured by XPS results in the characteristic background to photoemission peaks obvious in survey spectra. The production of inelastic scattered electrons is modelled by an exponential decay in zero loss photoemission recorded. Intensity for electrons emerging from a layer within the surface is obtained by integrating the signal over the interval $[p, q]$ using the exponential attenuation model $\boldsymbol{e}^{-x/a}$ for the reduction in intensity at the surface due to photoemission at a depth x beneath the surface. The value for a determines the sampling depth for photoemission from a specific material at a specific energy for a photoelectron.



The intensity emitted at the surface I from a layer of material between the depths of p and q is proportional to the integral:

$$I \propto \int_{p}^{q} e^{-x/a}\, dx = a\left[e^{-p/a} - e^{-q/a}\right]$$

For $p = 0$ and $q = 3a$ then 95% of photoemission signal without energy loss is accounted for from the surface layer, hence the sampling depth for XPS is often referred to a three times the effective attenuation length. When considering the upper energies for Al anode x-ray emission the value for a is between 3 and 4 nm, hence a common rule of thumb is that for Al x-rays the maximum sampling depth is in the region of 10 nm.

The value a for photoemission from solid state materials varies as a function of kinetic energy of the electrons detected. Even for a sample of uniform depth distribution such as gold, silver or copper, the number of electrons recorded for an emission peak reduces as the energy of the electrons decreases simply because the volume of material from which an electron can emerge without inelastic scattering reduces.

For a given analysis area, the volume of material sampled for a given kinetic energy for the emitted electrons can be modelled using the Inelastic Mean Free Path (IMFP) λ or Effective Attenuation Length (EAL). Martin Seah publish universal equation approximations to IMPF (λ) and EAL

$$\lambda = \frac{(0.73 + 0.0095E^{0.872})}{Z^{0.3}} \quad (nm)$$

$$EAL = \frac{(0.65 + 0.007E^{0.93})}{Z^{0.38}} \quad (nm)$$

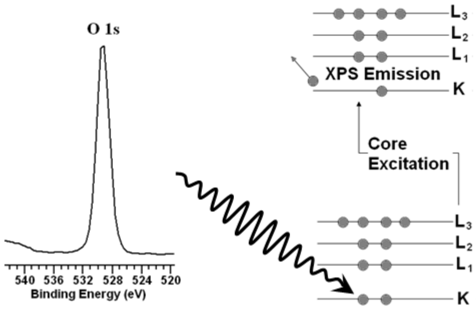
where E is the photoelectron kinetic energy and Z is the average atomic number provide a means of correcting for escape depth dependence on kinetic energy.

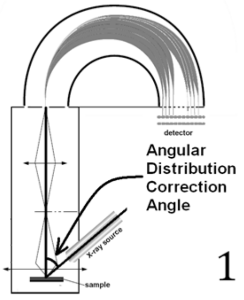
XPS data only offers the possibility for reporting the amount of substance when properly corrected emission peaks are used in the atomic concentration formula applied to truly homogeneous samples.

Quantification by XPS Illustrate using Fused Silica

Relative Sensitivity Factor
Scofield Cross-Sections

Instrument Geometry





For Magic Angle
Instruments Angular
Distribution Correction is
Not Required

$$1 - \frac{\beta}{4}\left(3\cos^2\theta - 1\right)$$

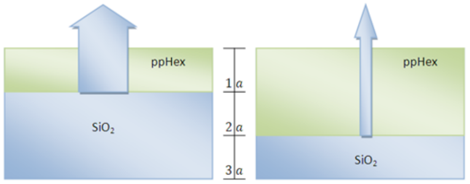
Approximation (Martin Seah) to IMFP (λ) and EAL

$$\lambda = \frac{(0.73 + 0.0095E^{0.872})}{Z^{0.3}} \quad (nm)$$

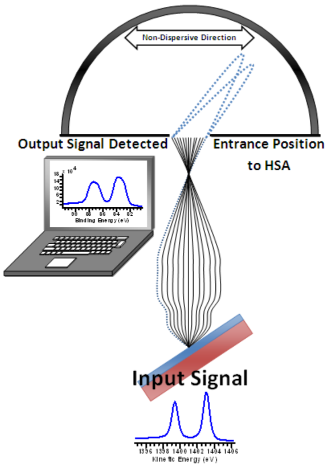
$$EAL = \frac{(0.65 + 0.007E^{0.93})}{Z^{0.38}} \quad (nm)$$

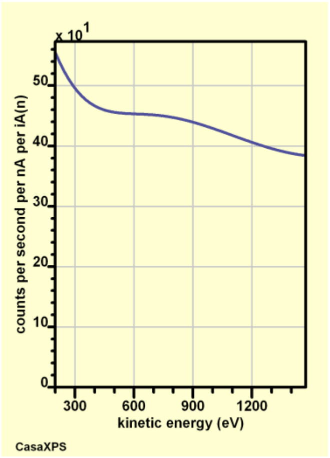
E is the photoelectron kinetic energy

Z is the average atomic number



$$I \propto \int_p^q e^{-x/a}\,dx = a\left[e^{-p/a} - e^{-q/a}\right]$$

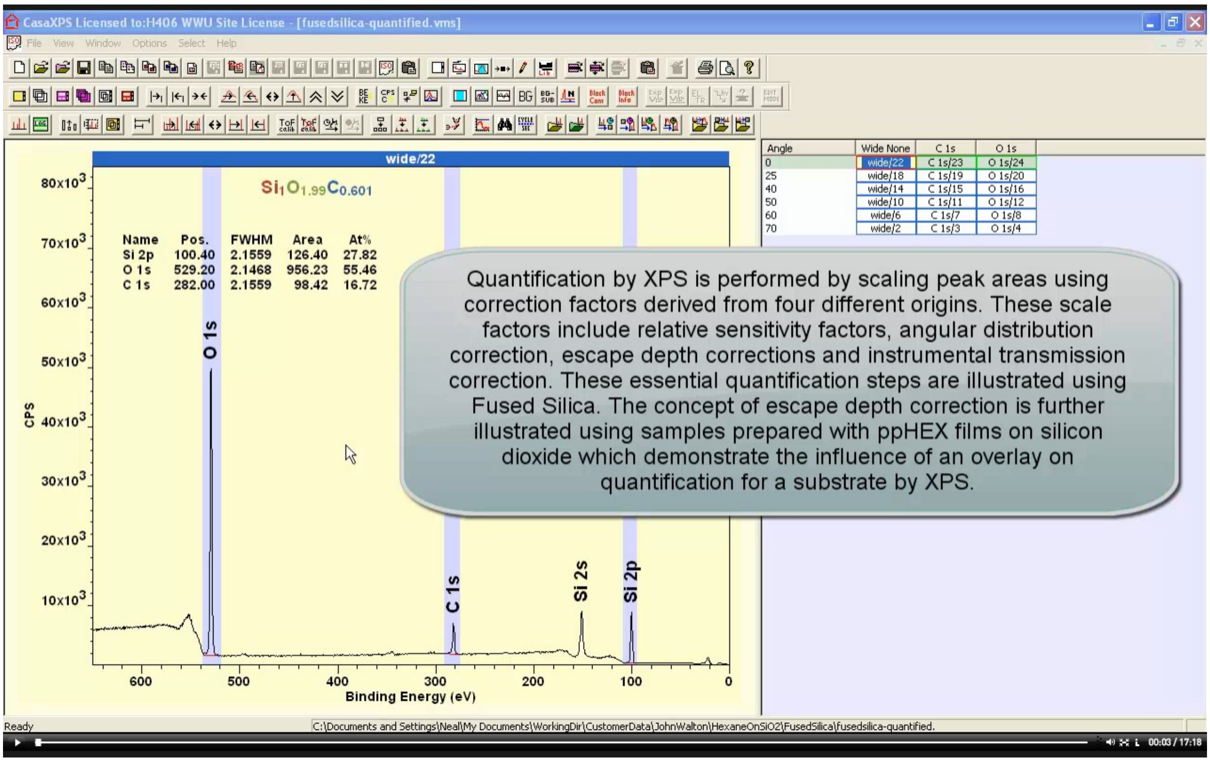




The basic tools used to assess sample chemistry are quantification regions defined for isolated photoemission peaks. In the case of fused silica photoemission peaks corresponding to Si 2p, O 1s and C 1s are isolated from any interfering photoemission peaks. As a consequence quantification regions can be used to define appropriate approximations to inelastic scattered background signal, intervals over which signal above the inelastic scatter background is integrated to yield raw counts per second eV (CPSeV) for each peak. These raw CPSeV are then scaled using relative sensitivity factors in the form of Scofield cross-sections, which are adjusted for angular distribution based on an angle of 60° between the axis of the analysers lens column and the Al anode X-ray source. Escape depth correction is performed using the EAL approximation to allow for differences between the sampling depths for O 1s and Si 2p signal. Finally instrument response to kinetic energy is corrected by making use of a transmission function computed for these data using the NPL transmission correction procedure.

In principle, the computed transmission function effectively allows recorded data to appear as if it were measured from an instrument created with ideal flat transmission response to electron photoemission energy. Only when a precise transmission correction is available is the use of Scofield cross-sections appropriate. Another way of looking at this statement is, in principle, any instrument for which relative sensitivity factors are other than Scofield cross-sections does not have an absolute and true transmission function available.

Fused Silica Video

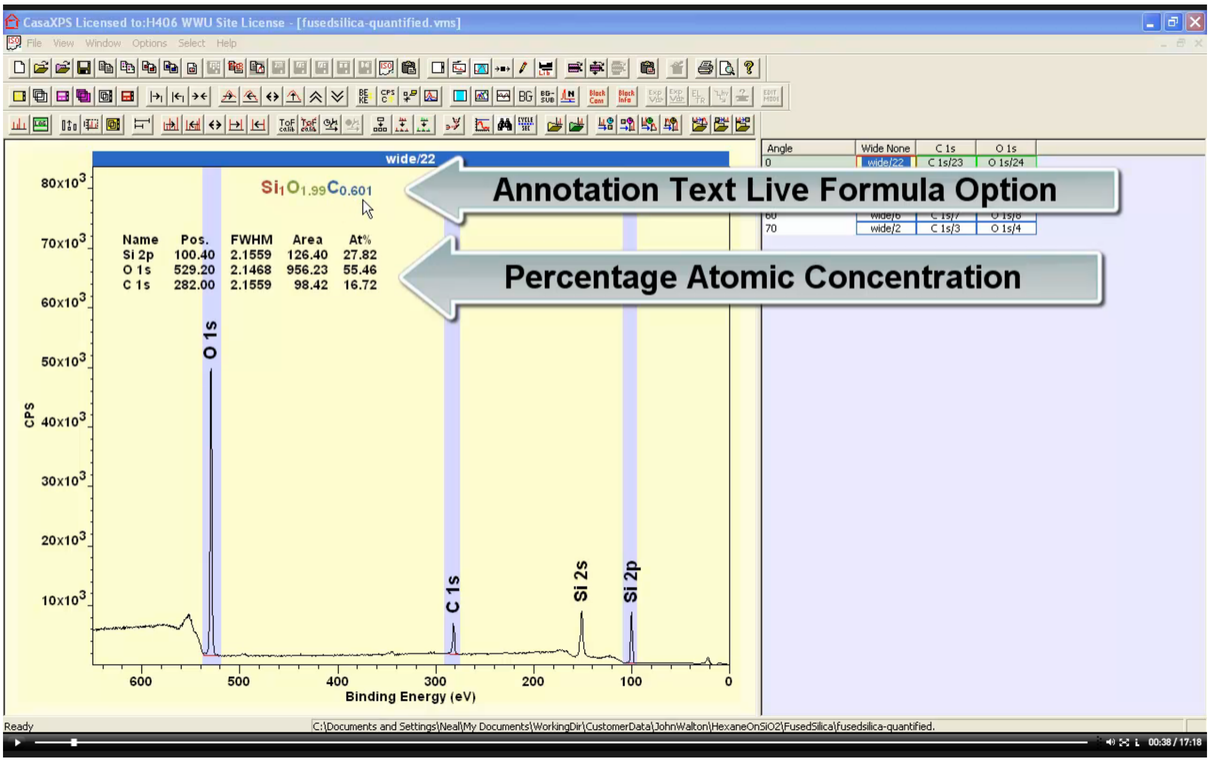


Name	Pos.	FWHM	Area	At%
Si 2p	100.40	2.1559	126.40	27.82
O 1s	529.20	2.1468	956.23	55.46
C 1s	282.00	2.1559	98.42	16.72

Angle	Wide None	C 1s	O 1s
0	wide/22	C 1s/23	O 1s/24
25	wide/18	C 1s/19	O 1s/20
40	wide/14	C 1s/15	O 1s/16
50	wide/10	C 1s/11	O 1s/12
60	wide/6	C 1s/7	O 1s/8
70	wide/2	C 1s/3	O 1s/4

Quantification by XPS is performed by scaling peak areas using correction factors derived from four different origins. These scale factors include relative sensitivity factors, angular distribution correction, escape depth corrections and instrumental transmission correction. These essential quantification steps are illustrated using Fused Silica. The concept of escape depth correction is further illustrated using samples prepared with ppHEX films on silicon dioxide which demonstrate the influence of an overlay on quantification for a substrate by XPS.

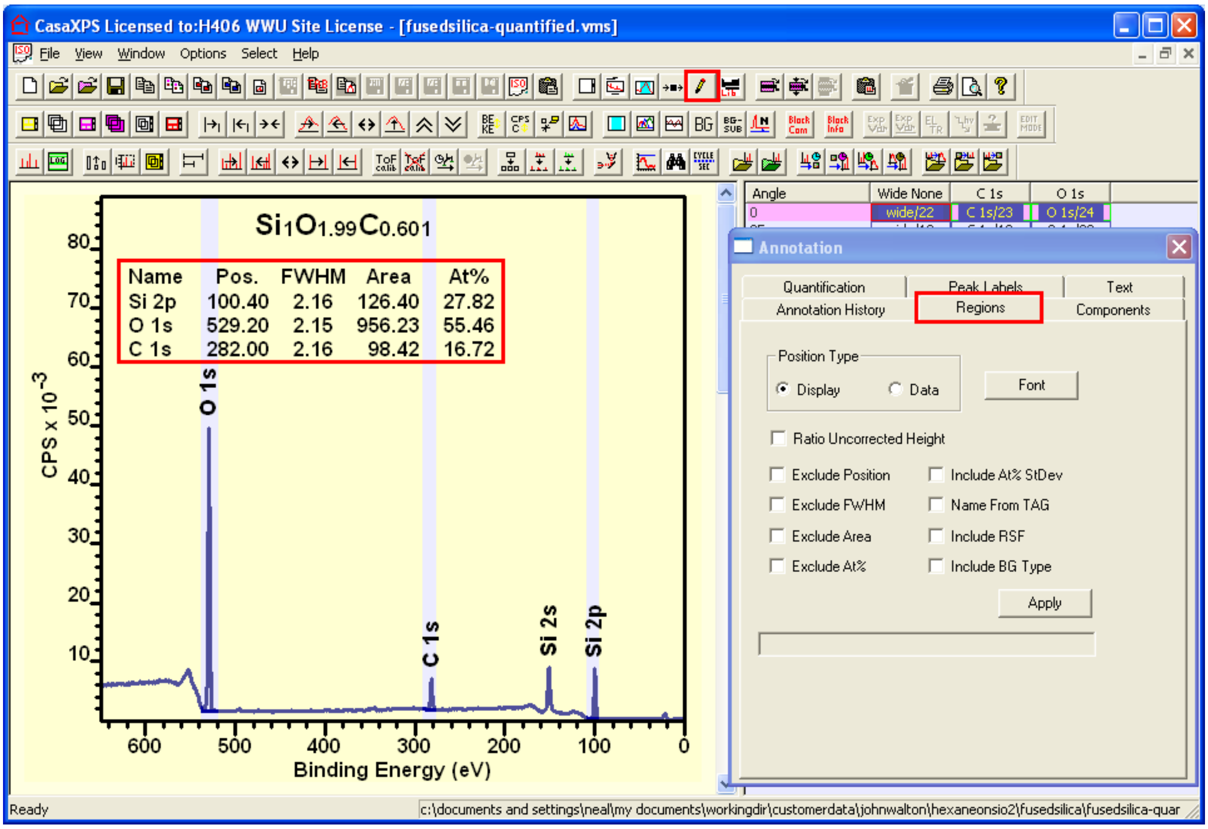
Quantification steps used to transform raw survey spectra into stoichiometric relationships between silicon and oxygen are explain for a sample expected to be fused silica.



Name	Pos.	FWHM	Area	At%
Si 2p	100.40	2.1559	126.40	27.82
O 1s	529.20	2.1468	956.23	55.46
C 1s	282.00	2.1559	98.42	16.72

Angle	Wide None	C 1s	O 1s
0	wide/22	C 1s/23	O 1s/24
70	wide/2	C 1s/3	O 1s/4

Quantification results from regions are display over data by adding annotation using the Annotation Dialog Regions property page table specification and the Formula option on the Annotation Dialog Text property page.



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$Si_1O_{1.99}C_{0.601}$

Name	Pos.	FWHM	Area	At%
Si 2p	100.40	2.16	126.40	27.82
O 1s	529.20	2.15	956.23	55.46
C 1s	282.00	2.16	98.42	16.72

Position Type: ● Display ○ Data

☐ Ratio Uncorrected Height

☐ Exclude Position
☐ Exclude FWHM
☐ Exclude Area
☐ Exclude At%
☐ Include At% StDev
☐ Name From TAG
☐ Include RSF
☐ Include BG Type

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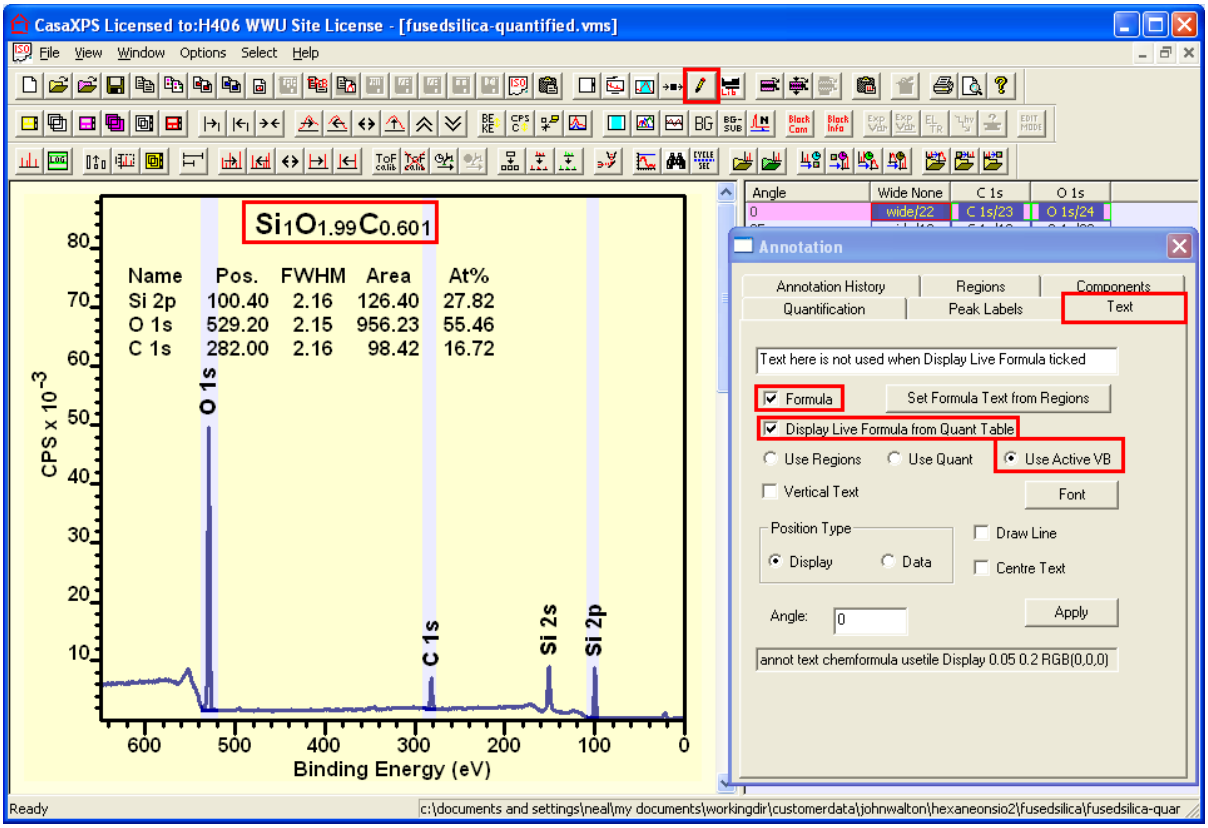
Annotation dialog Regions property page.



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$Si_1O_{1.99}C_{0.601}$

Name	Pos.	FWHM	Area	At%
Si 2p	100.40	2.16	126.40	27.82
O 1s	529.20	2.15	956.23	55.46
C 1s	282.00	2.16	98.42	16.72

Text here is not used when Display Live Formula ticked

☑ Formula

☑ Display Live Formula from Quant Table

○ Use Regions ○ Use Quant ● Use Active VB

☐ Vertical Text

Position Type: ● Display ○ Data

☐ Draw Line

☐ Centre Text

Angle: 0

annot text chemformula usetile Display 0.05 0.2 RGB(0,0,0)

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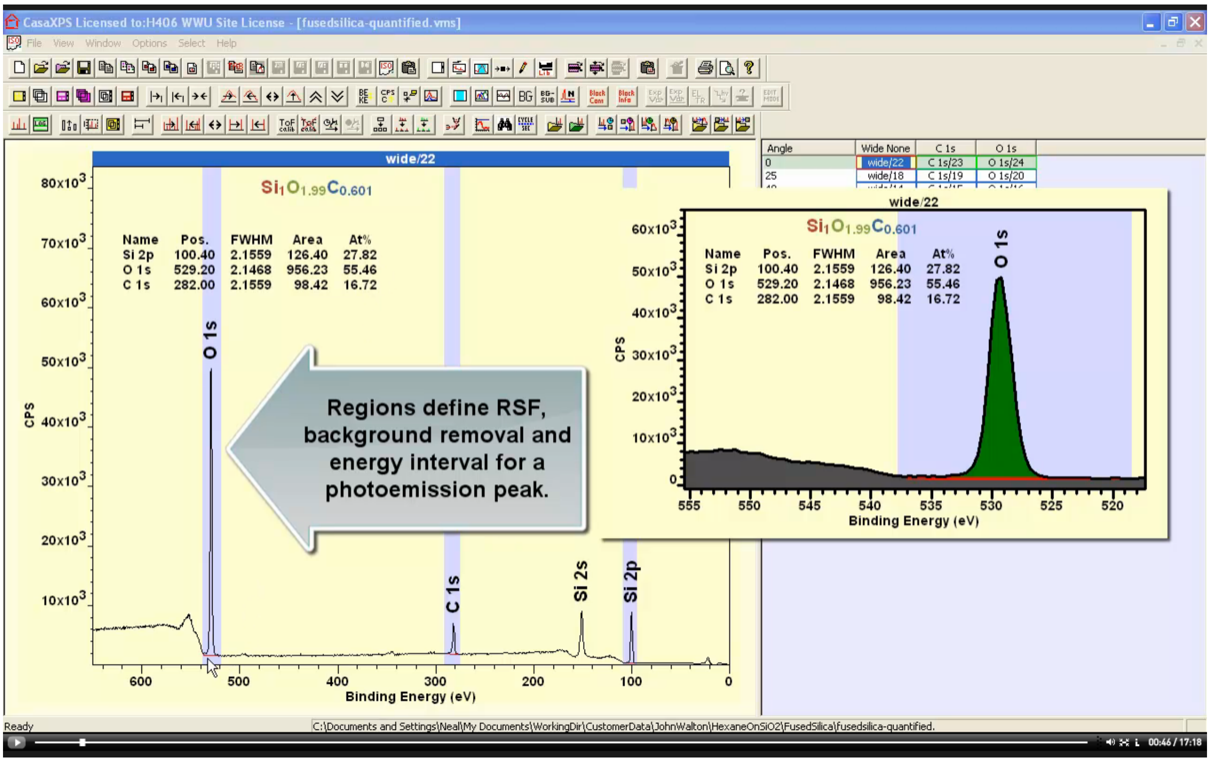
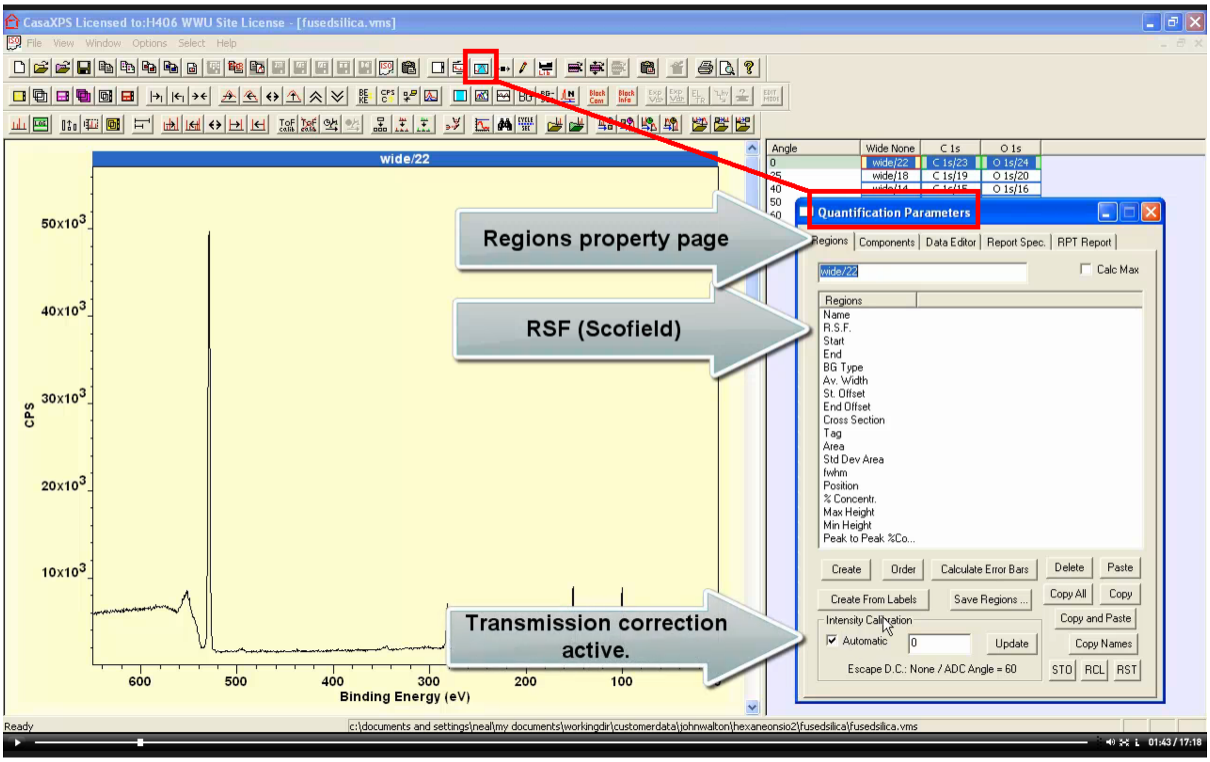
Annotation dialog Text property page making use of options for extracting the displayed text from quantification results gathered from regions.



$Si_1O_{1.99}C_{0.601}$

Name	Pos.	FWHM	Area	At%
Si 2p	100.40	2.1559	126.40	27.82
O 1s	529.20	2.1468	956.23	55.46
C 1s	282.00	2.1559	98.42	16.72

Regions define RSF, background removal and energy interval for a photoemission peak.



☑ Automatic 0

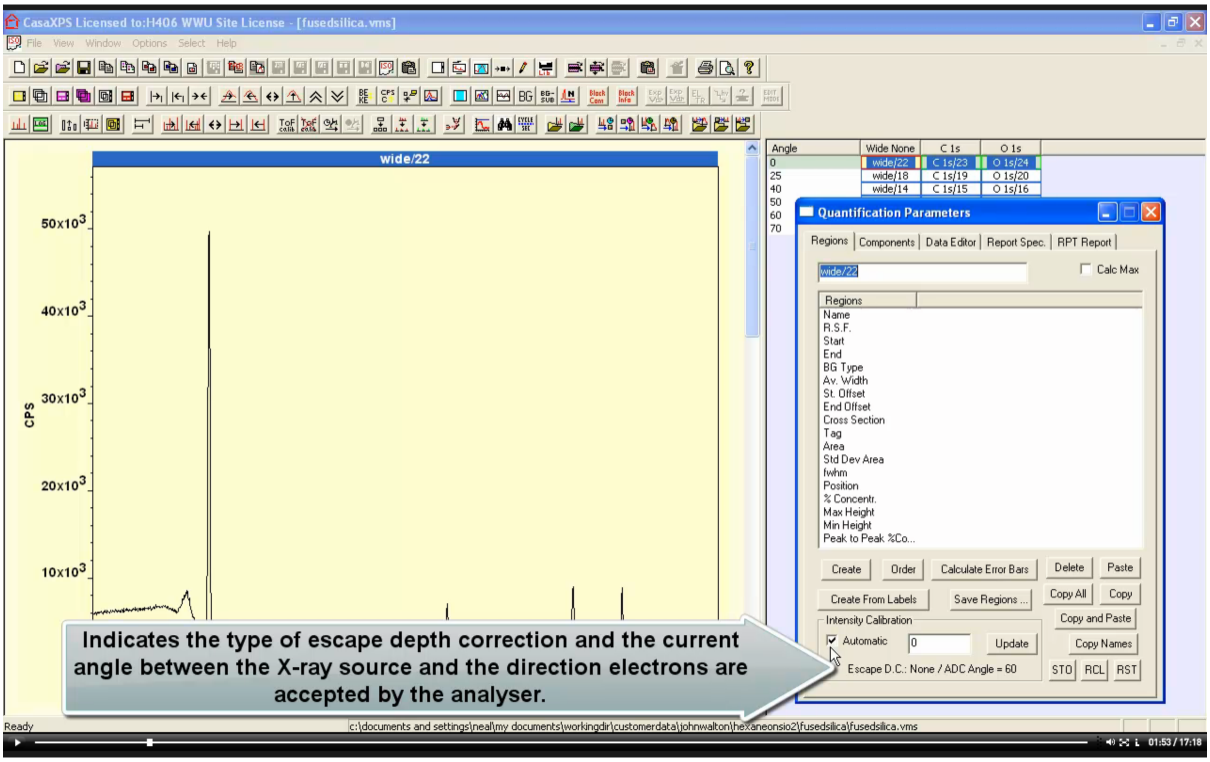
Escape D.C.: None / ADC Angle = 60

Regions property page

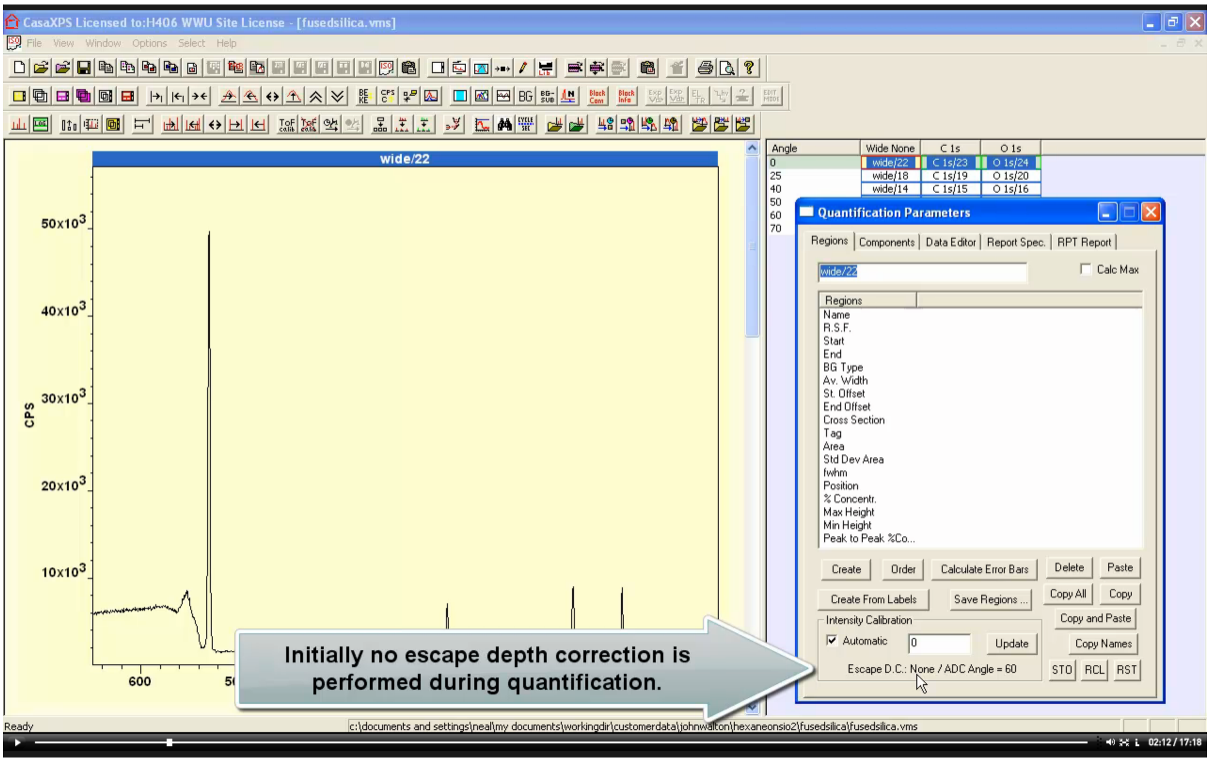
RSF (Scofield)

Transmission correction active.

The Quantification Parameters dialog window Regions property page allows the specification of quantification information specific to a photoemission peak (RSF, background and energy interval) and displays the currently active intensity calibration options in the form of transmission, escape depth and angular distribution corrections.

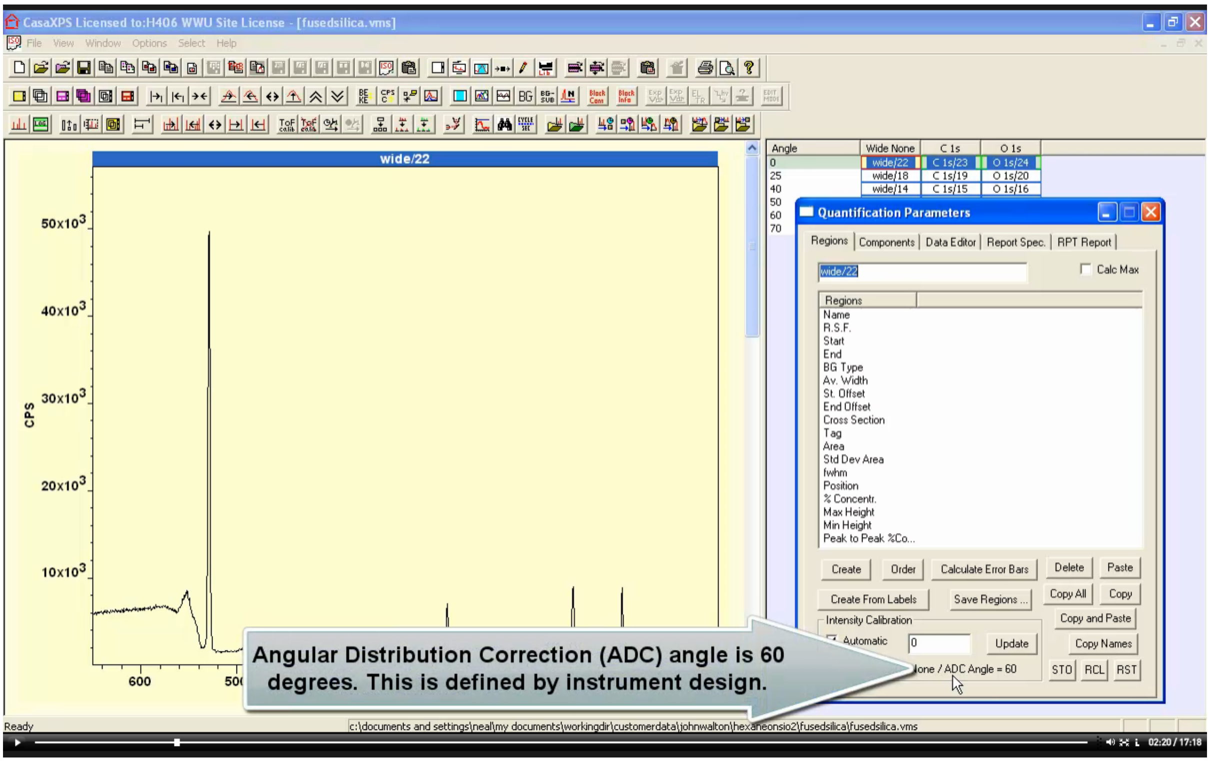


Indicates the type of escape depth correction and the current angle between the X-ray source and the direction electrons are accepted by the analyser.



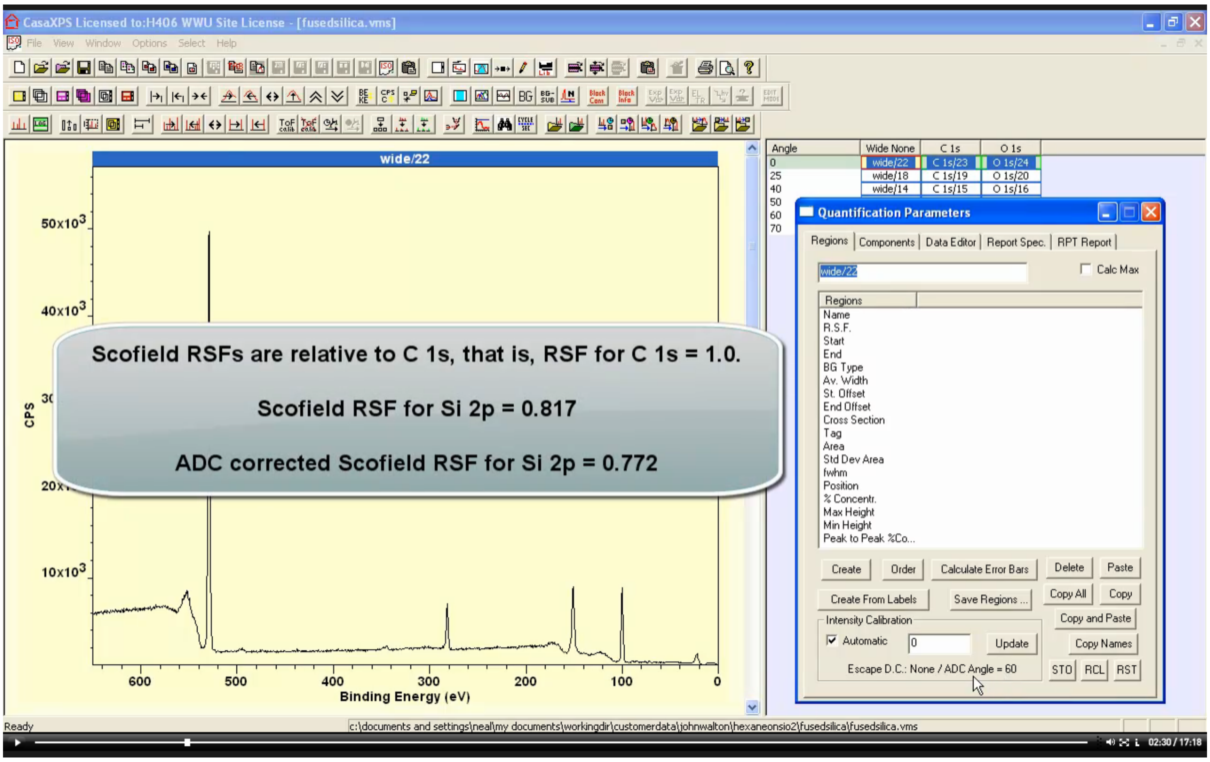
Initially no escape depth correction is performed during quantification.

During the course of this video quantification regions are defined and intensity calibration steps are progressively added resulting in traceable quantification for a fused silica sample. Initially transmission correction based on an NPL computed transmission function is active.



Angular Distribution Correction (ADC) angle is 60 degrees. This is defined by instrument design.

Angular distribution correction is active too making use of an angle of 60° between the direction for electrons collected by the transfer lens system and the x-ray source. ADC information is used to adjust the relative sensitivity factor for a region at the time a region is created.

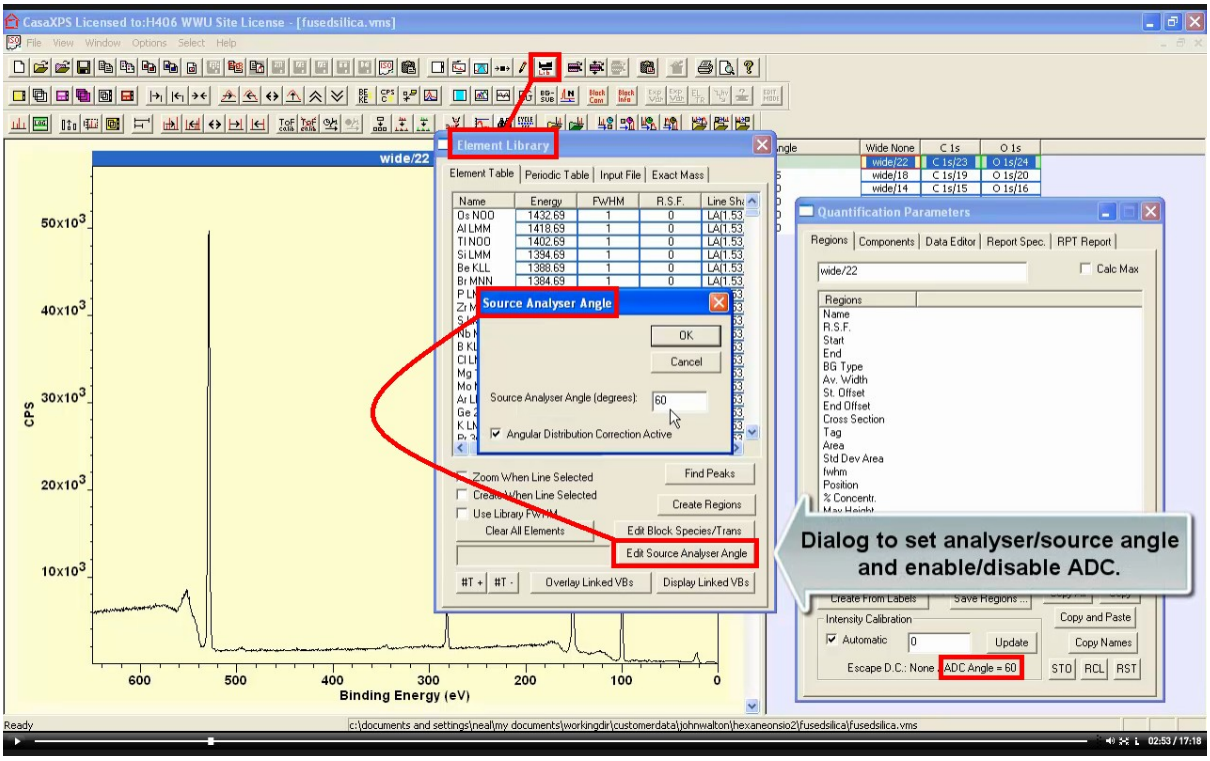


Scofield RSFs are relative to C 1s, that is, RSF for C 1s = 1.0.

Scofield RSF for Si 2p = 0.817

ADC corrected Scofield RSF for Si 2p = 0.772

The element library contains an RSF for Si 2p equal to 0.817. This value for the Si 2p RSF is computed by Scofield using quantum mechanics to compute the photoionisation cross-section for Al anode x-rays exciting a Si atom initially in the ground state.



Name	Energy	FWHM	R.S.F.	Line Sha
Os NOO	1432.69	1	0	LA(1.53
Al LMM	1418.69	1	0	LA(1.53
Tl NOO	1402.69	1	0	LA(1.53
Si LMM	1394.69	1	0	LA(1.53
Be KLL	1388.69	1	0	LA(1.53
Br MNN	1384.69	1	0	LA(1.53

Source Analyser Angle

Source Analyser Angle (degrees): 60

☑ Angular Distribution Correction Active

☐ Zoom When Line Selected

☐ Create When Line Selected

☐ Use Library FWHM

Wide None	C 1s	O 1s
wide/22	C 1s/23	O 1s/24
wide/18	C 1s/19	O 1s/20
wide/14	C 1s/15	O 1s/16

wide/22 ☐ Calc Max

Regions: Name, R.S.F., Start, End, BG Type, Av. Width, St. Offset, End Offset, Cross Section, Tag, Area, Std Dev Area, fwhm, Position, % Concentr., Max Height

Intensity Calibration

☑ Automatic 0

Escape D.C.: None ADC Angle = 60

Dialog to set analyser/source angle and enable/disable ADC.

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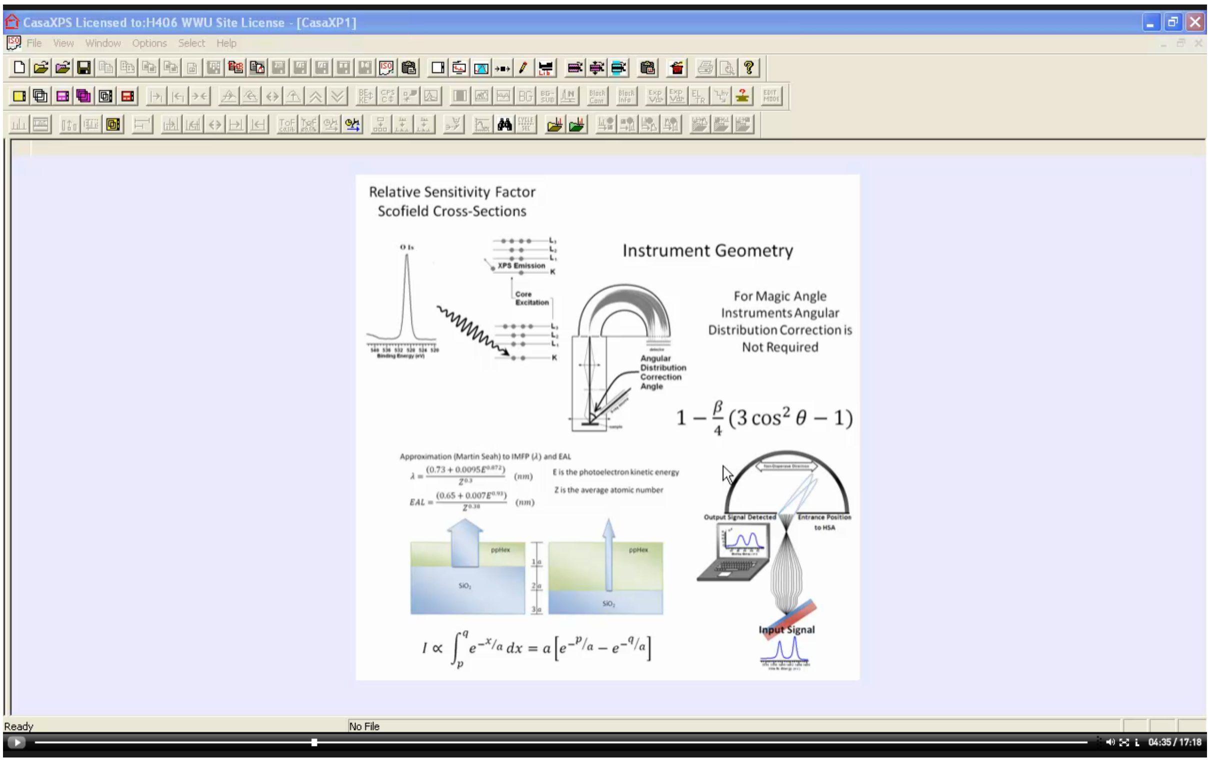
Values for the ADC angle can be adjusted using the Element Library dialog window Element Table property page.



Relative Sensitivity Factor
Scofield Cross-Sections

Instrument Geometry

For Magic Angle Instruments Angular Distribution Correction is Not Required

$$1 - \frac{\beta}{4}\left(3\cos^2\theta - 1\right)$$

Approximation (Martin Seah) to IMFP (λ) and EAL

$$\lambda = \frac{(0.73 + 0.0095E^{0.872})}{Z^{0.3}} \quad (nm)$$

$$EAL = \frac{(0.65 + 0.007E^{0.93})}{Z^{0.38}} \quad (nm)$$

E is the photoelectron kinetic energy

Z is the average atomic number

$$I \propto \int_p^q e^{-x/a}\,dx = a\left[e^{-p/a} - e^{-q/a}\right]$$

For each region a total sensitivity factor is computed based on Scofield RSF, transmission function for the photoemission energy, escape depth for the photoemission energy and the source analyser angle instrument geometry.

Research article

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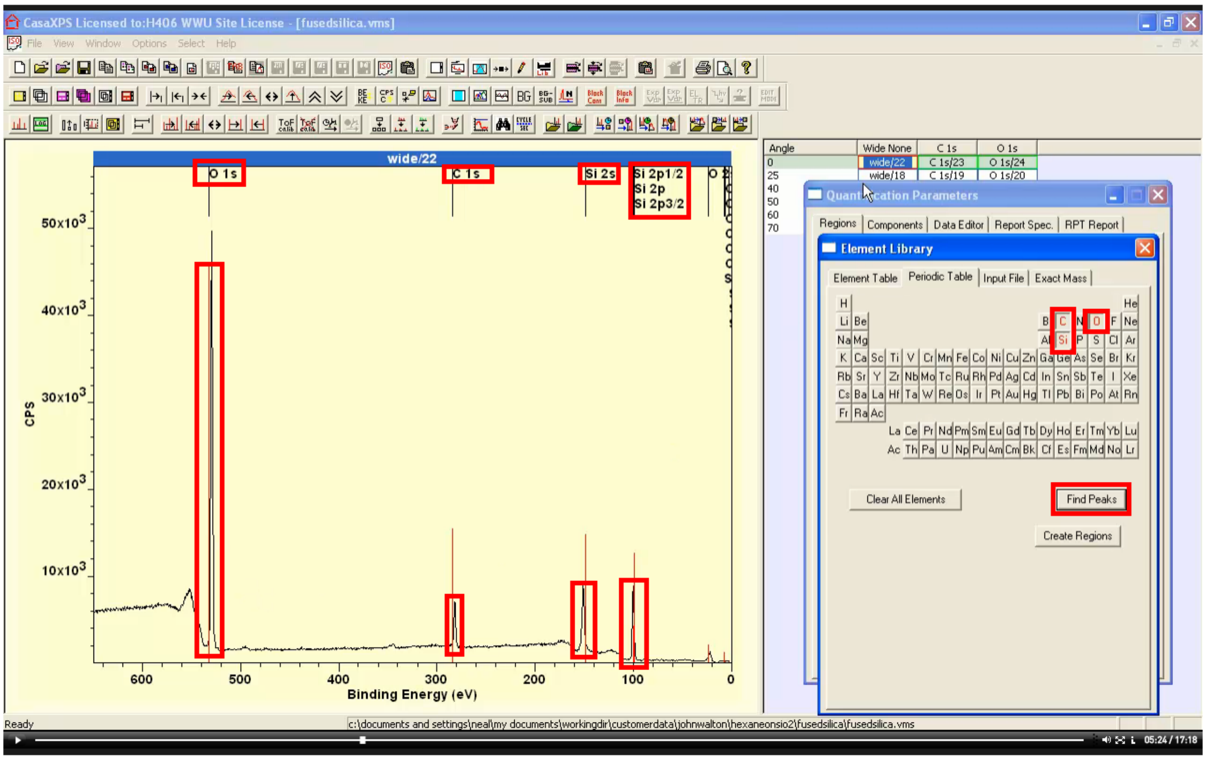
Film thickness measurement and contamination layer correction for quantitative XPS

J. Walton,[a*] M. R. Alexander,[b] N. Fairley,[c] P. Roach[d] and A. G. Shard[e]

In order to determine the most appropriate method of measuring film thickness using imaging XPS, a series of thin polymer films have been prepared and analysed using spectroscopy. The thickness of these thin polymer films has been determined using peak shape analysis and by using photoelectron peak areas compared with a bulk reference and by using relative sensitivity factors. These results have been compared with values obtained using ellipsometry. The values obtained by measuring photoelectron peak areas were seen to be influenced by the chemistry of the film, so that a bulk reference of similar chemistry to the film is required for accurate thickness measurement. The values obtained using peak shape analysis, both interactive and non-interactive, were not dependent on the chemistry of the film and showed good agreement with ellipsometry. Imaging of a patterned polymer film was successfully carried out, and the polymer cross section was shown to provide a reasonable description of the inelastic background from the carbonaceous contamination layer. An image of the substrate photoelectron intensity was successfully corrected for attenuation in both the carbonaceous contamination layer and the polymer film simultaneously using an image of the film thickness determined by non-interactive peak shape analysis. This procedure is suitable for automated film thickness measurement and correction for attenuation in the carbonaceous contamination layer in both spectroscopy and imaging. Copyright © 2016 John Wiley & Sons, Ltd.

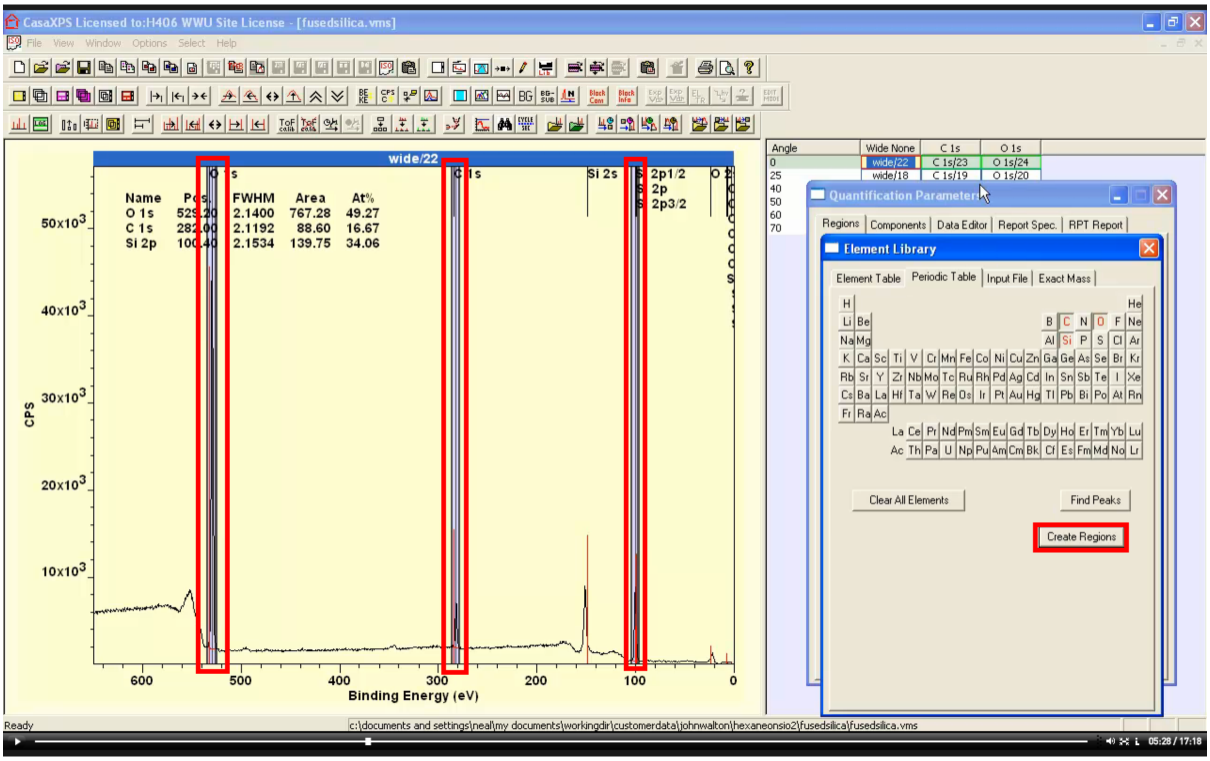
Keywords: XPS; imaging; film thickness; peak shape analysis; carbonaceous contamination

Information about escape depth corrections and how escape depth can be used to understand sample composition by XPS is described in Walton et al (SIA 2016).



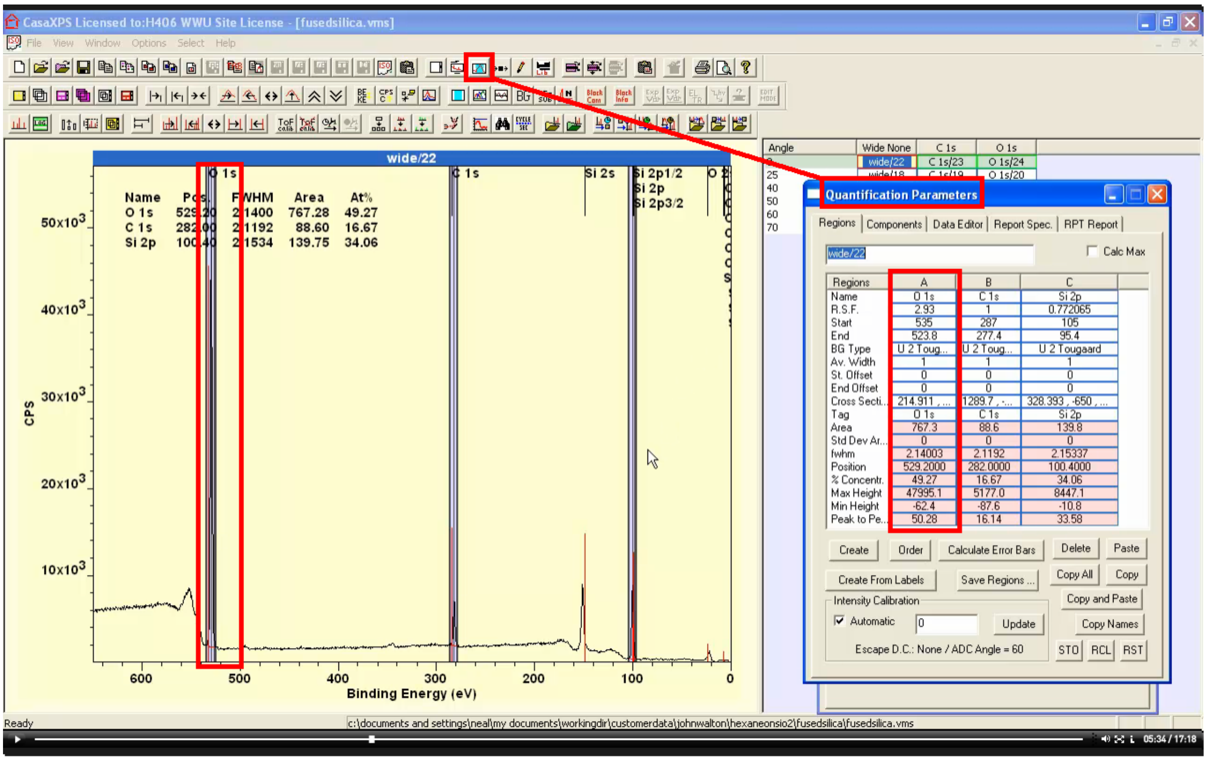
Angle	Wide None	C 1s	O 1s
0	wide/22	C 1s/23	O 1s/24
25	wide/18	C 1s/19	O 1s/20
40			
50			
60			
70			

Quantification regions can be created by marking each element of interest using the Element Library dialog window via the Element Table and Periodic Table property pages. The Find Peaks button marks any peak with element markers for which a possible match occurs. This is a superset of elements rather than attempting to identify the most likely.



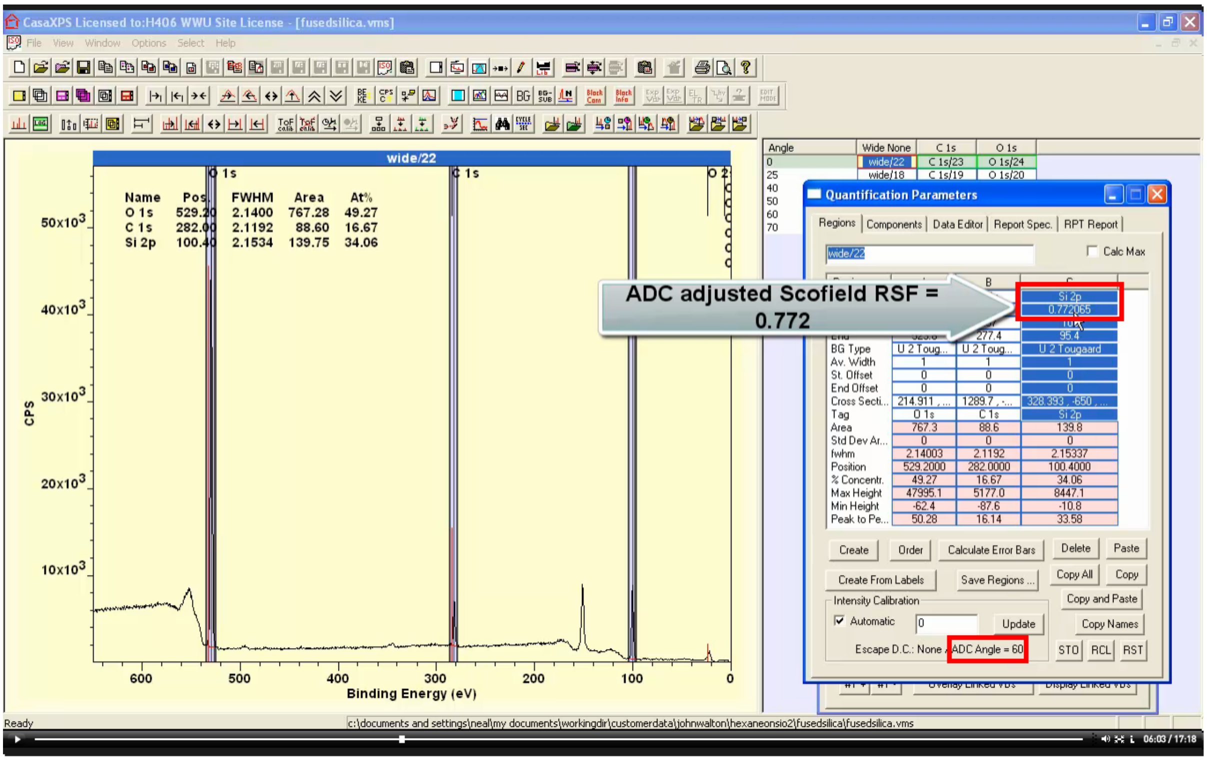
Name	Pos	FWHM	Area	At%
O 1s	529.20	2.1400	767.28	49.27
C 1s	282.00	2.1192	88.60	16.67
Si 2p	100.40	2.1534	139.75	34.06

Once the user assesses the superset of elements and limits the element markers to the most likely elements (in this case C 1s, O 1s and Si) regions are created using element markers by pressing the Create Regions button on the Periodic Table or Element Table property pages.



Regions	A	B	C
Name	O 1s	C 1s	Si 2p
R.S.F.	2.93	1	0.772065
Start	535	287	105
End	523.8	277.4	95.4
BG Type	U 2 Toug...	U 2 Toug...	U 2 Tougaard
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	214.911 , ...	1289.7 , -...	328.393 , -650 , ...
Tag	O 1s	C 1s	Si 2p
Area	767.3	88.6	139.8
Std Dev Ar...	0	0	0
fwhm	2.14003	2.1192	2.15337
Position	529.2000	282.0000	100.4000
% Concentr.	49.27	16.67	34.06
Max Height	47995.1	5177.0	8447.1
Min Height	-62.4	-87.6	-10.8
Peak to Pe...	50.28	16.14	33.58

Regions are created and can be edited using the Quantification Parameters dialog Regions property page.

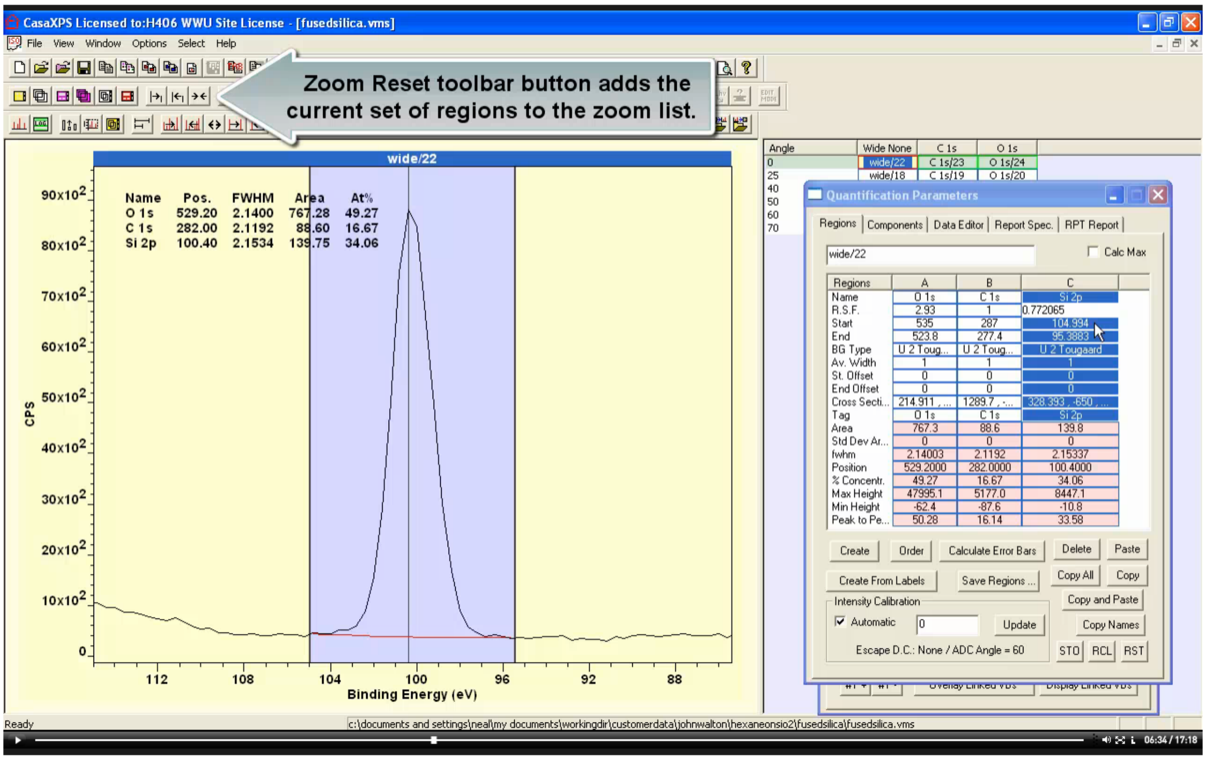


ADC adjusted Scofield RSF = 0.772

Name	Pos.	FWHM	Area	At%
O 1s	529.20	2.1400	767.28	49.27
C 1s	282.00	2.1192	88.60	16.67
Si 2p	100.40	2.1534	139.75	34.06

Regions	A	B	C
Name			Si 2p
R.S.F.			0.772065
End		277.4	95.4
BG Type	U 2 Toug...	U 2 Toug...	U 2 Tougaard
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	214.911 , ...	1289.7 , -...	328.393 , -650 , ...
Tag	O 1s	C 1s	Si 2p
Area	767.3	88.6	139.8
Std Dev Ar...	0	0	0
fwhm	2.14003	2.1192	2.15337
Position	529.2000	282.0000	100.4000
% Concentr.	49.27	16.67	34.06
Max Height	47995.1	5177.0	8447.1
Min Height	-62.4	-87.6	-10.8
Peak to Pe...	50.28	16.14	33.58

Note the Si 2p is the only region with an ADC corrected RSF. RSFs in the Scofield library are relative to C 1s sensitivity and ADC for electrons with s orbital angular momentum the correction is identical for all elements. Differences occur in ADC for p, d, f orbital angular momentum therefore the Si 2p RSF is the only RSF out of C 1s, O 1s and Si 2p that requires ADC adjustments.

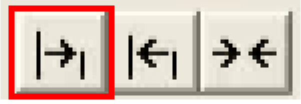


Zoom Reset toolbar button adds the current set of regions to the zoom list.

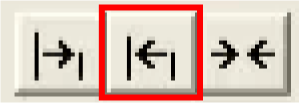
Name	Pos.	FWHM	Area	At%
O 1s	529.20	2.1400	767.28	49.27
C 1s	282.00	2.1192	88.60	16.67
Si 2p	100.40	2.1534	139.75	34.06

Regions	A	B	C
Name	O 1s	C 1s	Si 2p
R.S.F.	2.93	1	0.772065
Start	535	287	104.994
End	523.8	277.4	95.3883
BG Type	U 2 Toug...	U 2 Toug...	U 2 Tougaard
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	214.911 , ...	1289.7 , -...	328.393 , -650 , ...
Tag	O 1s	C 1s	Si 2p
Area	767.3	88.6	139.8
Std Dev Ar...	0	0	0
fwhm	2.14003	2.1192	2.15337
Position	529.2000	282.0000	100.4000
% Concentr.	49.27	16.67	34.06
Max Height	47995.1	5177.0	8447.1
Min Height	-62.4	-87.6	-10.8
Peak to Pe...	50.28	16.14	33.58

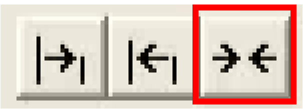
Each time a zoom action occurs the dimensions for the display in terms of energy and intensity intervals is added to a zoom list. Toolbar buttons allow the zoom states to be used to view data in sequence. When regions are defined on a VAMAS block and the Reset zoom list toolbar button is pressed the energy intervals defined by the current set of regions is used to initialise the zoom list. Cycling through the zoom list allows each region to be viewed in turn.



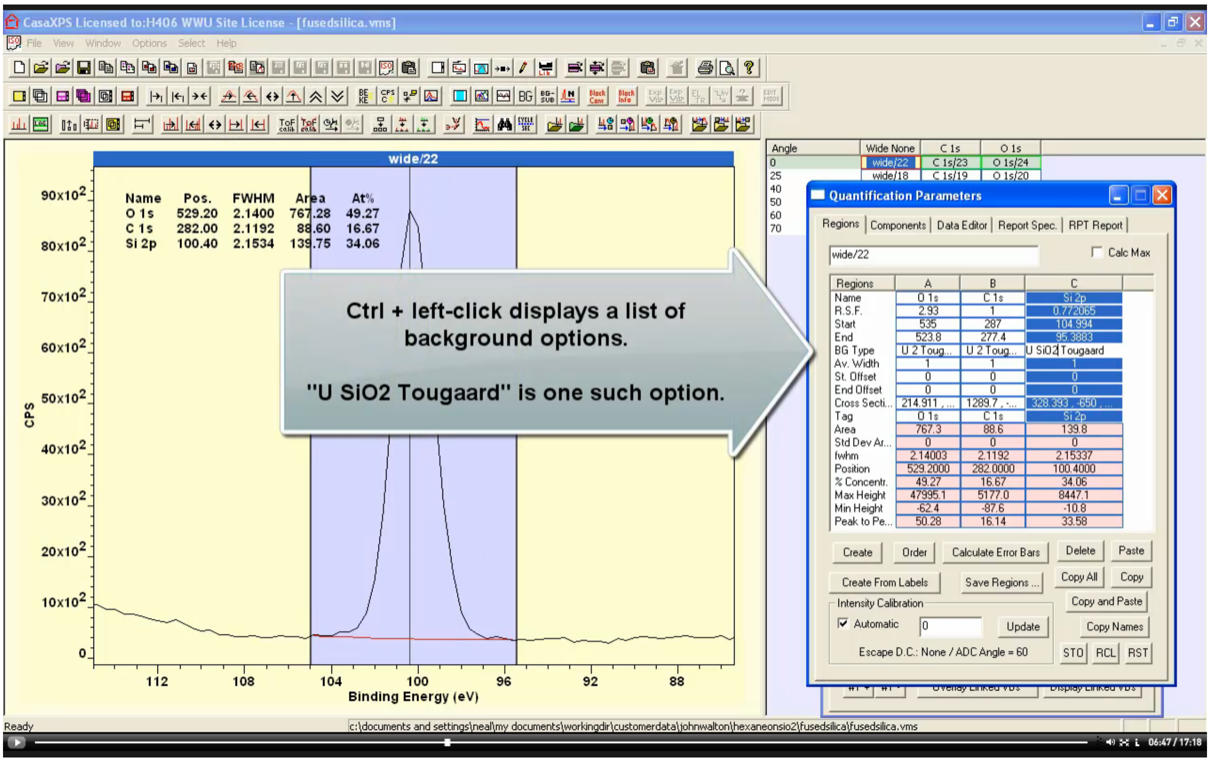
Zoom In toolbar button creates a new zoom state using a box drawn using the mouse and the left mouse button to drag a box over the left hand display tile. The new zoom state is added to the current zoom list.



Zoom Out toolbar button steps through the zoom states currently active for the left hand display tile. The set of current zoom state are cycled through repeatedly by pressing the Zoom Out toolbar button.



Reset Zoom List toolbar button will empty the zoom list or if regions are defined on the active spectrum in the active display tile, energy intervals defined by these regions are added to the zoom list to allow the easy inspection of newly created region limits.



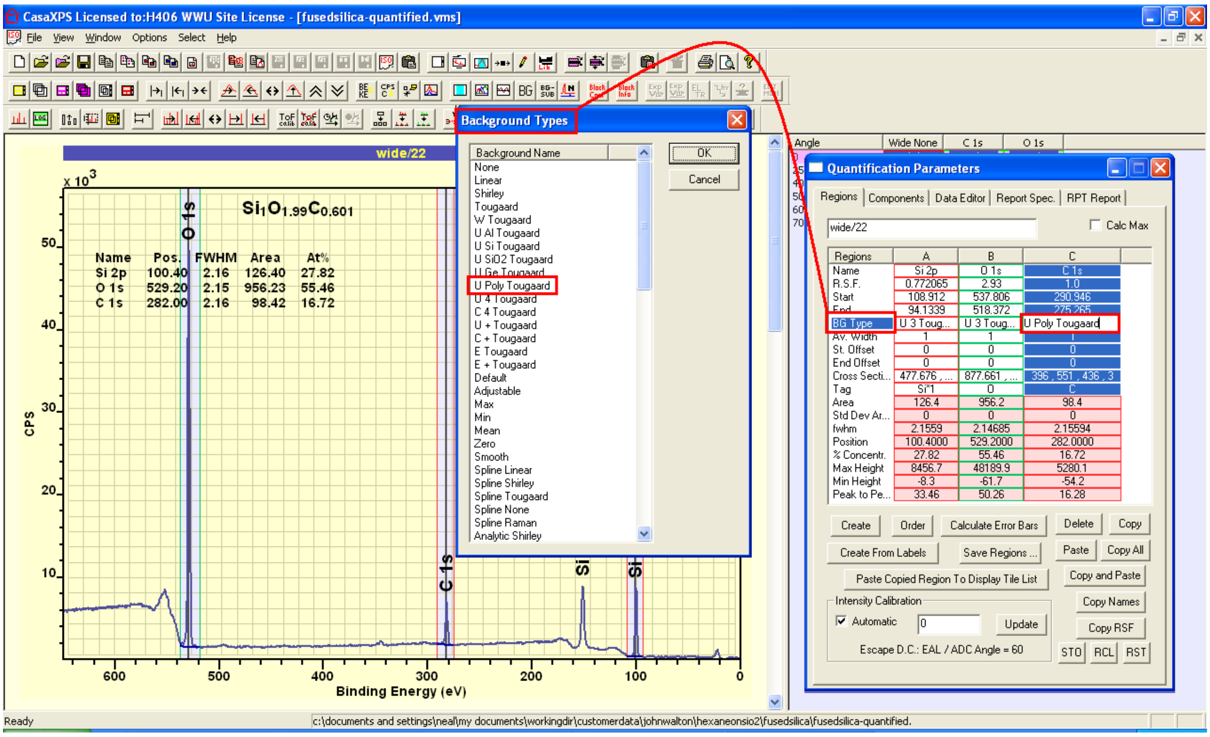
Name	Pos.	FWHM	Area	At%
O 1s	529.20	2.1400	767.28	49.27
C 1s	282.00	2.1192	88.60	16.67
Si 2p	100.40	2.1534	139.75	34.06

Ctrl + left-click displays a list of background options.

"U SiO2 Tougaard" is one such option.

Regions	A	B	C
Name	O 1s	C 1s	Si 2p
R.S.F.	2.93	1	0.772065
Start	535	287	104.994
End	523.8	277.4	95.3883
BG Type	U 2 Toug...	U 2 Toug...	U SiO2 Tougaard
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	214.911 , ...	1289.7 , -...	328.393 , -650 , ...
Tag	O 1s	C 1s	Si 2p
Area	767.3	88.6	139.8
Std Dev Ar...	0	0	0
fwhm	2.14003	2.1192	2.15337
Position	529.2000	282.0000	100.4000
% Concentr.	49.27	16.67	34.06
Max Height	47995.1	5177.0	8447.1
Min Height	-62.4	-87.6	-10.8
Peak to Pe...	50.28	16.14	33.58

BG Type refers to the type of approximation used to remove inelastic scattered background signal from intensity due to primary zero-loss photoemission signal used to quantify sample composition. There are many background types available including basic linear, Shirley and Universal Tougaard backgrounds, however there are more sophisticated backgrounds for materials such as fused silica established by Tougaard. These can be viewed and selected via a dialog window associated with the BG Type field within a region specification.



$Si_1O_{1.99}C_{0.601}$

Name	Pos.	FWHM	Area	At%
Si 2p	100.40	2.16	126.40	27.82
O 1s	529.20	2.15	956.23	55.46
C 1s	282.00	2.16	98.42	16.72

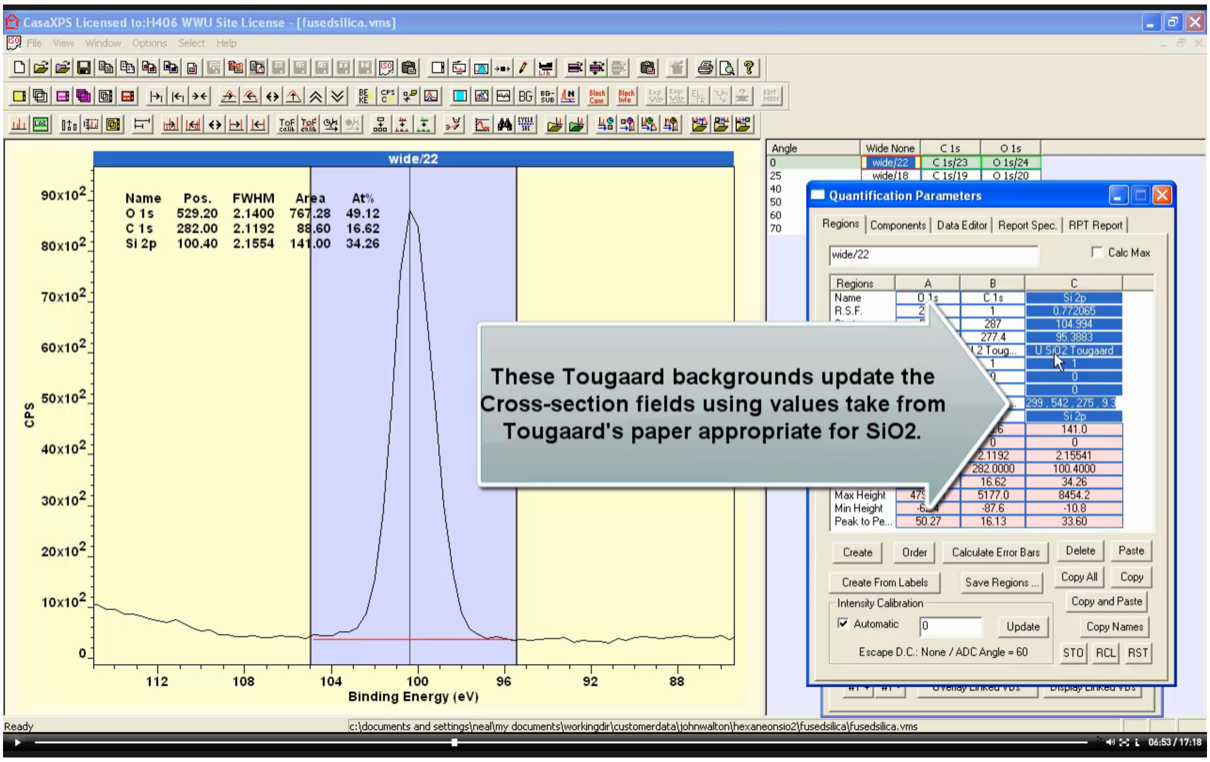
wide/22

☐ Calc Max

Regions	A	B	C
Name	Si 2p	O 1s	C 1s
R.S.F.	0.772065	2.93	1.0
Start	108.912	537.806	290.946
End	94.1339	518.372	275.265
BG Type	U 3 Toug...	U 3 Toug...	U Poly Tougaard
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	477.676 , ...	877.661 , ...	396 , 551 , 436 , 3
Tag	Si*1	O	C
Area	126.4	956.2	98.4
Std Dev Ar...	0	0	0
fwhm	2.1559	2.14685	2.15594
Position	100.4000	529.2000	282.0000
% Concentr.	27.82	55.46	16.72
Max Height	8456.7	48189.9	5280.1
Min Height	-8.3	-61.7	-54.2
Peak to Pe...	33.46	50.26	16.28

☑ Automatic 0

New features in CasaXPS 2.3.22 invoke the Background Type dialog window by selecting a BG Type field for an existing region before left clicking on the BG Type label within the Regions property page table of region parameters.

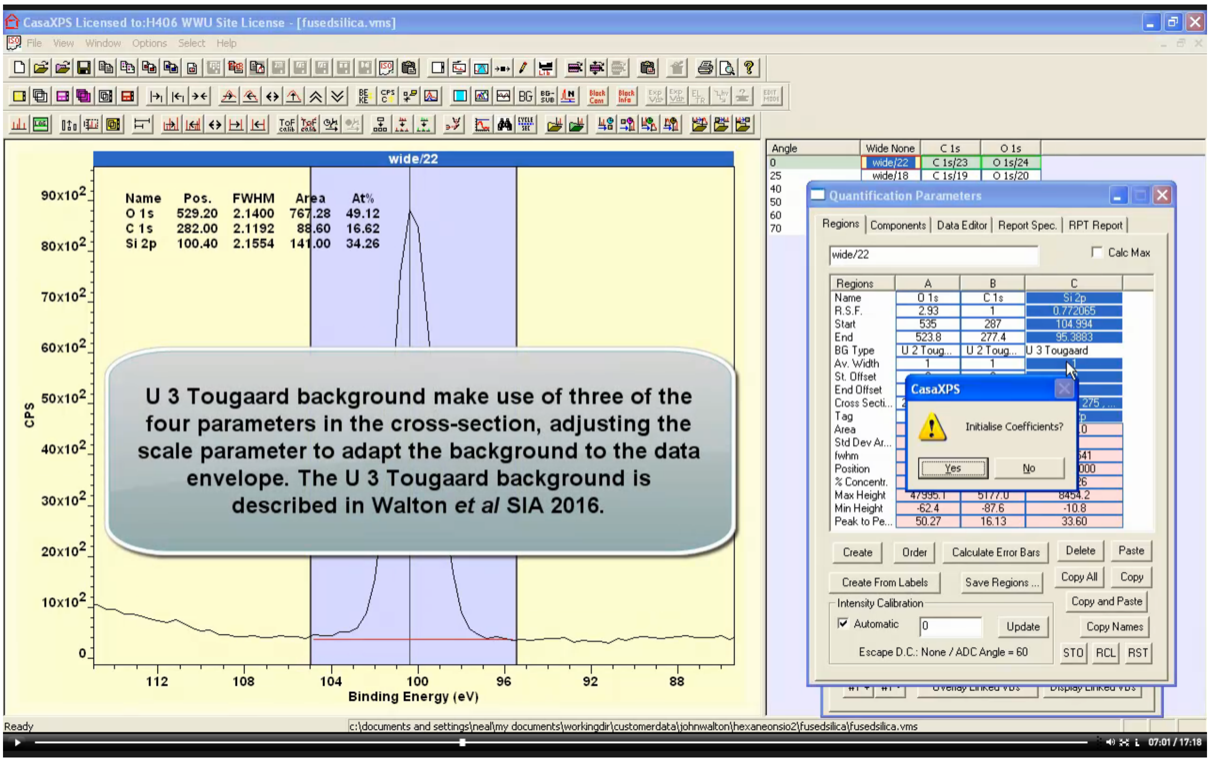


Name	Pos.	FWHM	Area	At%
O 1s	529.20	2.1400	767.28	49.12
C 1s	282.00	2.1192	88.60	16.62
Si 2p	100.40	2.1554	141.00	34.26

These Tougaard backgrounds update the Cross-section fields using values take from Tougaard's paper appropriate for SiO2.

Regions	A	B	C
Name	O 1s	C 1s	Si 2p
R.S.F.	2	1	0.772065
		287	104.994
		277.4	95.3883
		2 Toug...	U SiO2 Tougaard
		1	1
		0	0
			0
			299 , 542 , 275 , 9.3
			Si 2p
		6	141.0
		0	0
		2.1192	2.15541
		282.0000	100.4000
		16.62	34.26
Max Height	47	5177.0	8454.2
Min Height	-6	-87.6	-10.8
Peak to Pe...	50.27	16.13	33.60

After a specific Tougaard background type is selected, the cross-section field is updated with four parameters defined by Tougaard. The values for U SiO2 Tougaard are entered in the cross-section field. The cross-section functional form for the U 3 Tougaard background type is identical to the U SiO2 Tougaard cross-section however when the background type is set to U 3 Tougaard the cross-section fields can be manually adjusted, if required, and the B cross-section parameter is automatically computed for the specific interval of spectra defined by the region.



Name	Pos.	FWHM	Area	At%
O 1s	529.20	2.1400	767.28	49.12
C 1s	282.00	2.1192	88.60	16.62
Si 2p	100.40	2.1554	141.00	34.26

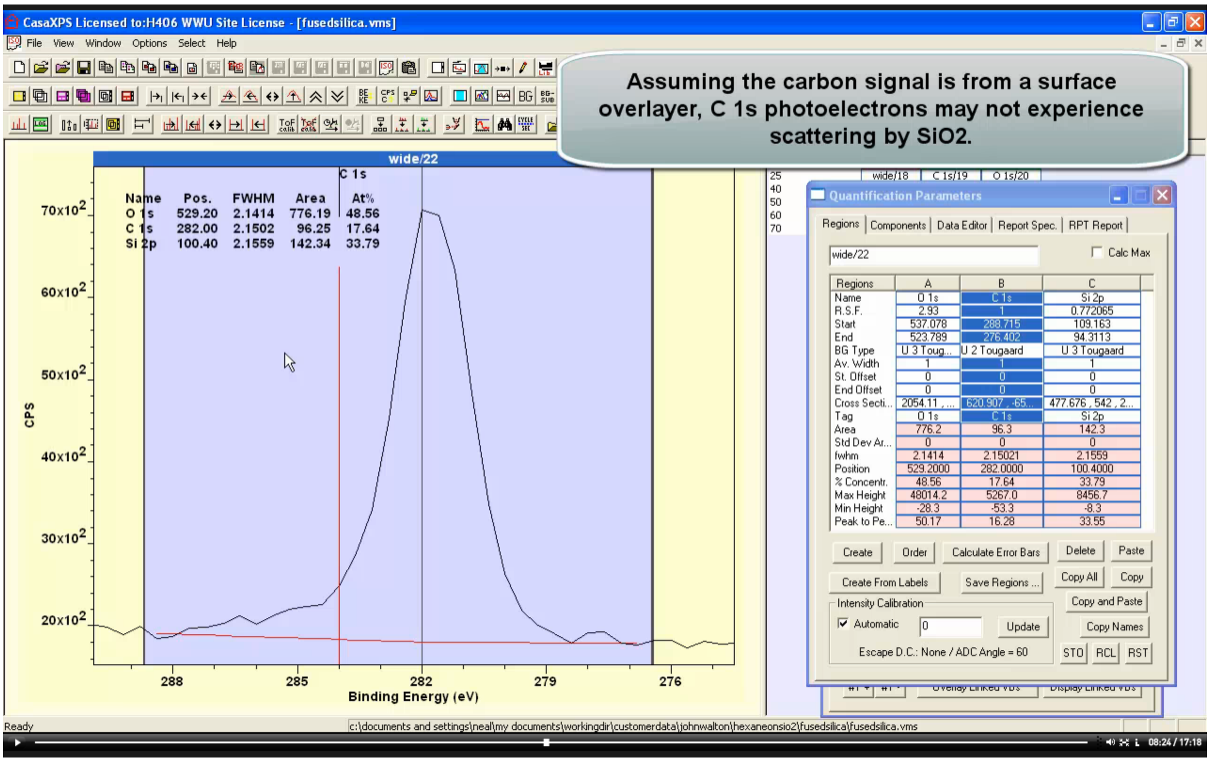
U 3 Tougaard background make use of three of the four parameters in the cross-section, adjusting the scale parameter to adapt the background to the data envelope. The U 3 Tougaard background is described in Walton *et al* SIA 2016.

wide/22

Regions	A	B	C
Name	O 1s	C 1s	Si 2p
R.S.F.	2.93	1	0.772065
Start	535	287	104.994
End	523.8	277.4	95.3883
BG Type	U 2 Toug...	U 2 Toug...	U 3 Tougaard
Av. Width	1	1	1
St. Offset			
End Offset			
Cross Secti...			
Tag			
Area			
Std Dev Ar...			
fwhm			
Position			
% Concentr.			
Max Height	47995.1	5177.0	8454.2
Min Height	-62.4	-87.6	-10.8
Peak to Pe...	50.27	16.13	33.60

Initialise Coefficients?

When the BG Type is changed from U SiO2 Tougaard to U 3 Tougaard a dialog window asks if the cross-section coefficients should be initialised. Since the U SiO2 Tougaard cross-section values are already appropriate for these data, the reply is to select the No button.



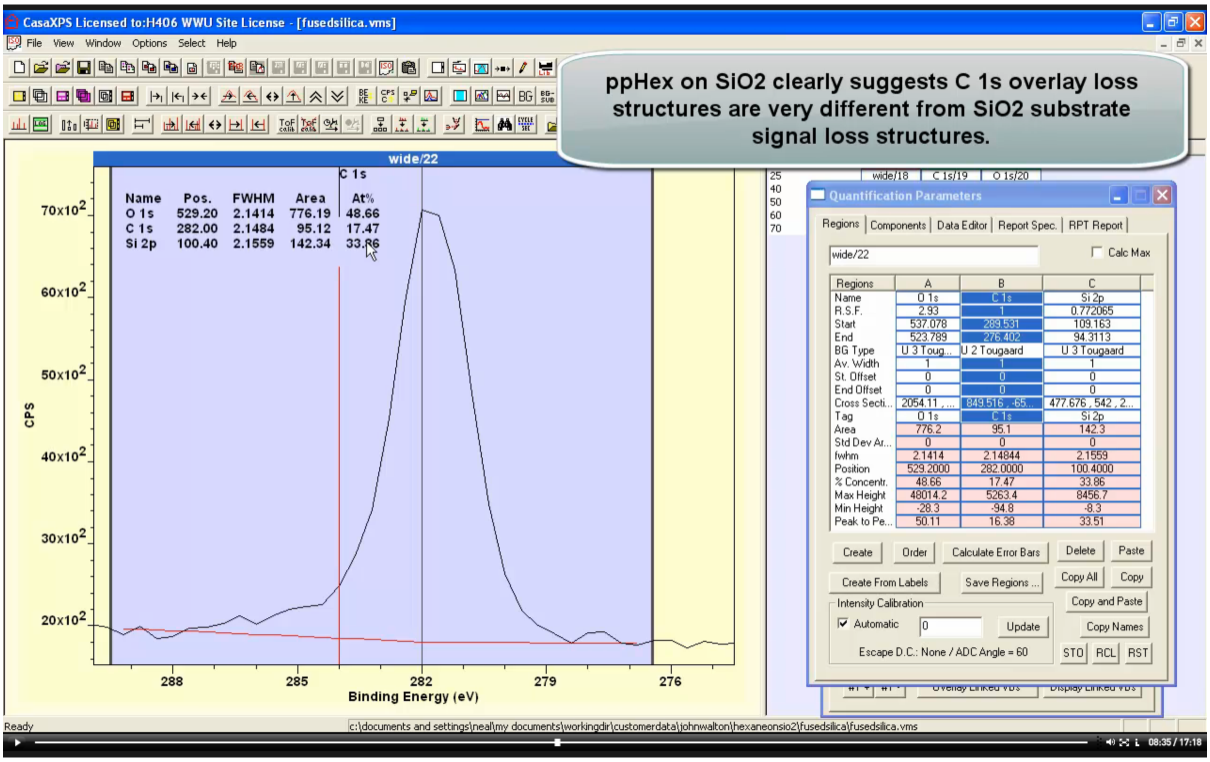
Assuming the carbon signal is from a surface overlayer, C 1s photoelectrons may not experience scattering by SiO2.

Name	Pos.	FWHM	Area	At%
O 1s	529.20	2.1414	776.19	48.56
C 1s	282.00	2.1502	96.25	17.64
Si 2p	100.40	2.1559	142.34	33.79

wide/22

Regions	A	B	C
Name	O 1s	C 1s	Si 2p
R.S.F.	2.93	1	0.772065
Start	537.078	288.715	109.163
End	523.789	276.402	94.3113
BG Type	U 3 Toug...	U 2 Tougaard	U 3 Tougaard
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	2054.11 , ...	620.907 , -65...	477.676 , 542 , 2...
Tag	O 1s	C 1s	Si 2p
Area	776.2	96.3	142.3
Std Dev Ar...	0	0	0
fwhm	2.1414	2.15021	2.1559
Position	529.2000	282.0000	100.4000
% Concentr.	48.56	17.64	33.79
Max Height	48014.2	5267.0	8456.7
Min Height	-28.3	-53.3	-8.3
Peak to Pe...	50.17	16.28	33.55

Inelastic scattering of photoelectrons depends on the material through which these electrons must pass en route to the vacuum. Photoemission from a surface contamination layer may experience different scattering events to those from a substrate. We assume for fused silica carbon is an overlay to SiO_2 and therefore only Si and O signal experiences scattering by Si and O electrons bond to these elements. C 1s signal is predominantly scattered by carbon atoms so may require a different background to Si 2p and O 1s peaks.

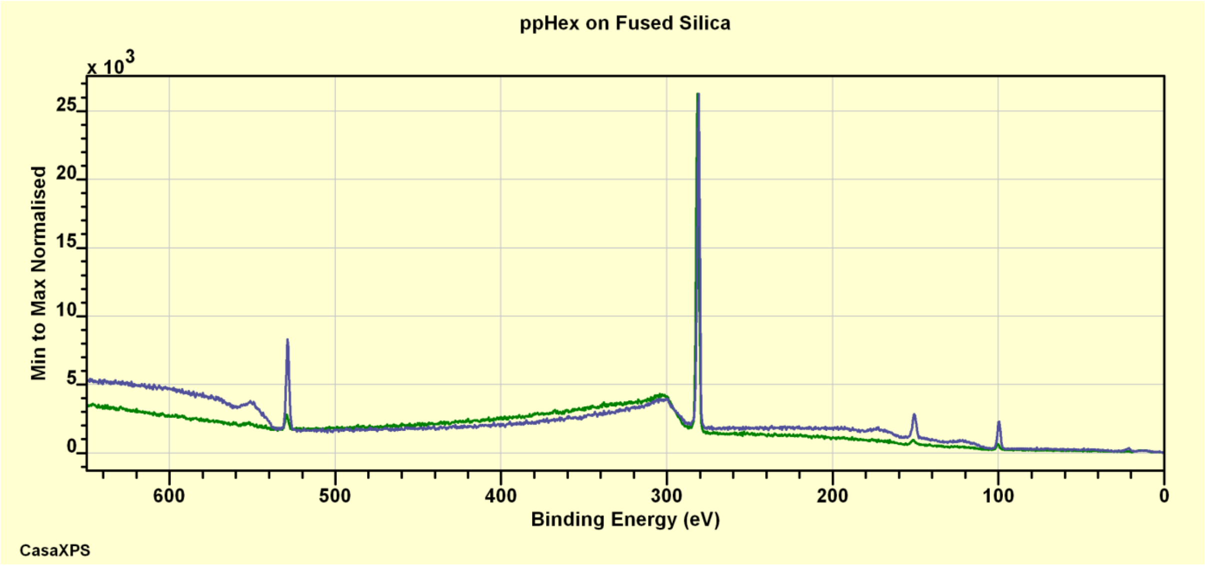


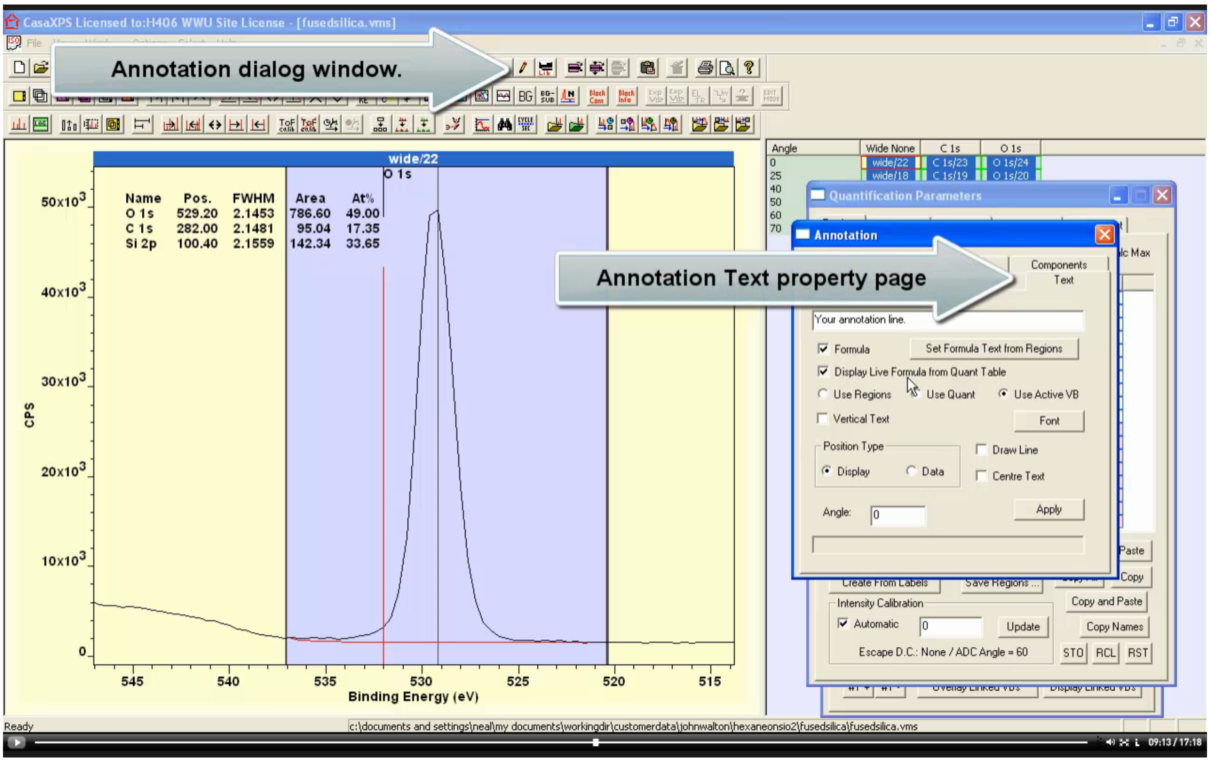
ppHex on SiO2 clearly suggests C 1s overlay loss structures are very different from SiO2 substrate signal loss structures.

Name	Pos.	FWHM	Area	At%
O 1s	529.20	2.1414	776.19	48.66
C 1s	282.00	2.1484	95.12	17.47
Si 2p	100.40	2.1559	142.34	33.86

Regions	A	B	C
Name	O 1s	C 1s	Si 2p
R.S.F.	2.93	1	0.772065
Start	537.078	289.531	109.163
End	523.789	276.402	94.3113
BG Type	U 3 Toug...	U 2 Tougaard	U 3 Tougaard
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	2054.11 , ...	849.516 , -65...	477.676 , 542 , 2...
Tag	O 1s	C 1s	Si 2p
Area	776.2	95.1	142.3
Std Dev Ar...	0	0	0
fwhm	2.1414	2.14844	2.1559
Position	529.2000	282.0000	100.4000
% Concentr.	48.66	17.47	33.86
Max Height	48014.2	5263.4	8456.7
Min Height	-28.3	-94.8	-8.3
Peak to Pe...	50.11	16.38	33.51

Backgrounds for these data are not important as both SiO_2 and carbon contamination result in relatively flat backgrounds beneath photoemission peaks. The significance of the background becomes more apparent when heterogeneous materials are analysed such as a layer of plasma-polymerised hexane on SiO_2.



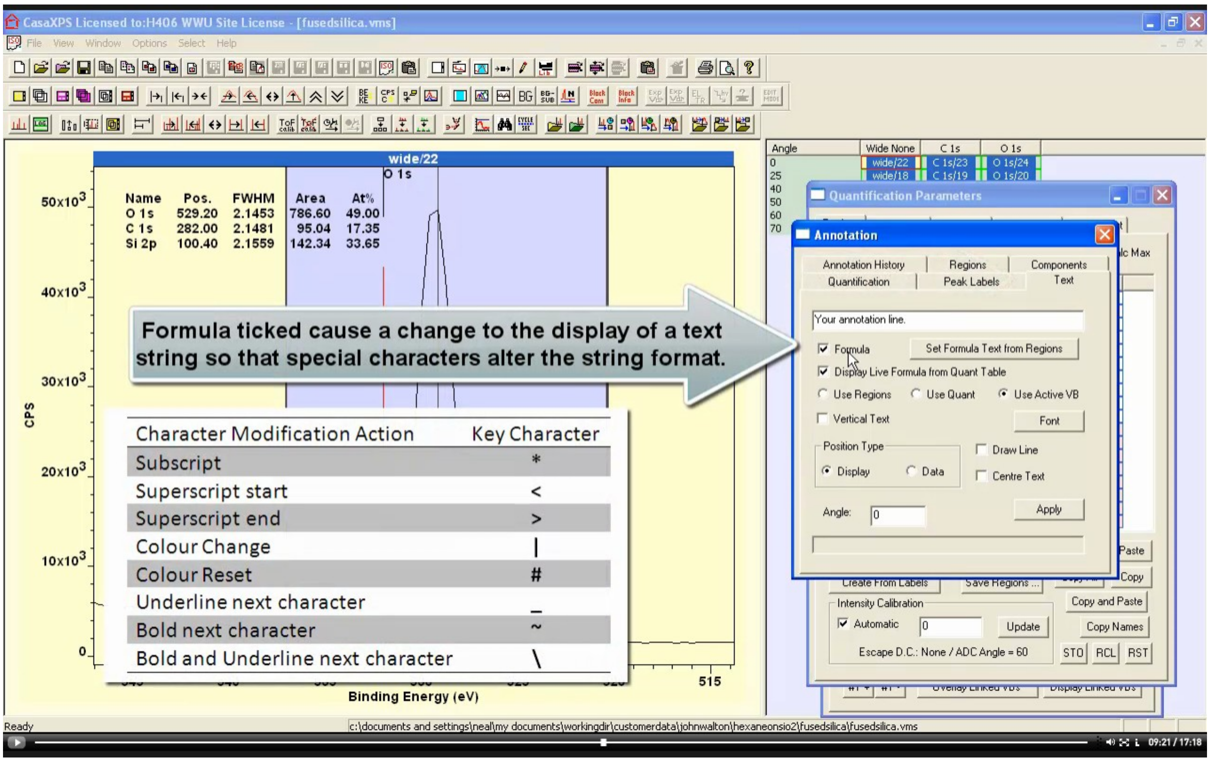


Annotation dialog window.

Annotation Text property page

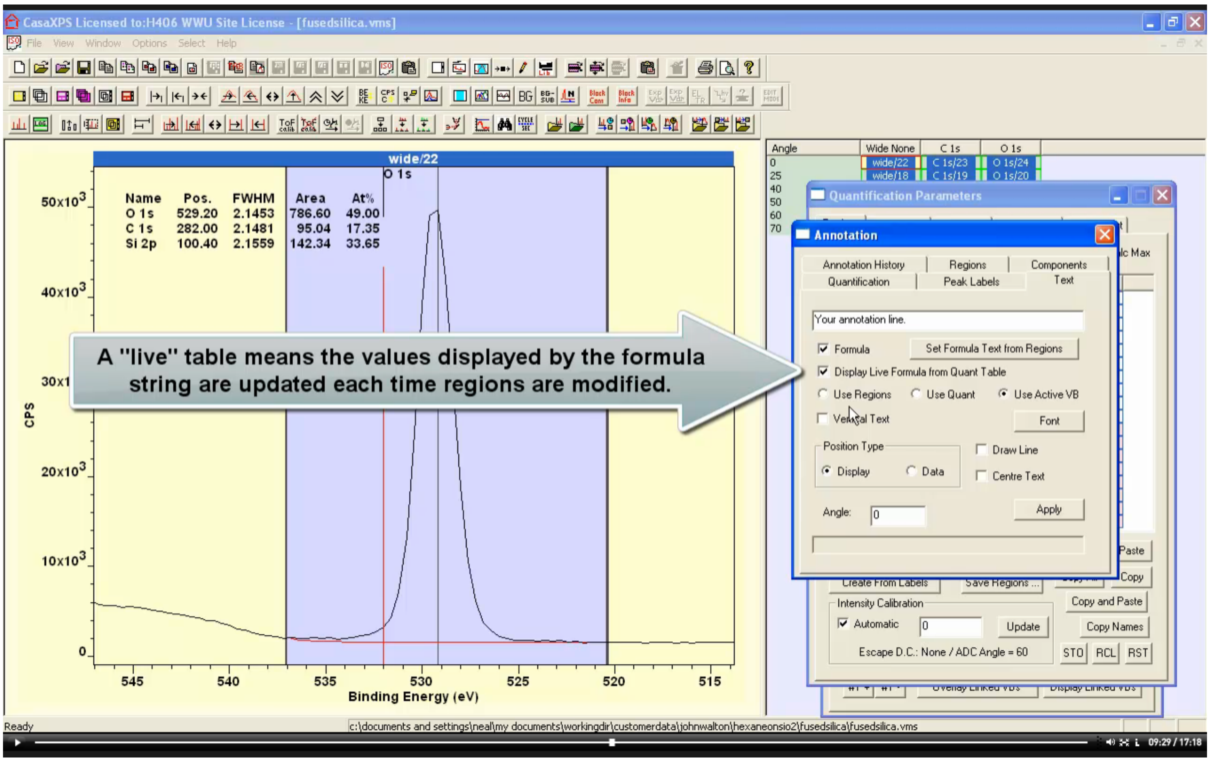
Name	Pos.	FWHM	Area	At%
O 1s	529.20	2.1453	786.60	49.00
C 1s	282.00	2.1481	95.04	17.35
Si 2p	100.40	2.1559	142.34	33.65

An alternative perspective to atomic concentration when viewing sample composition based on regions is the use of an option on the Annotation dialog window Text property page. The Formula option allows text to be displayed using subscripts and other formatting defined by expressions involving element symbols explicitly entered on the property page.



Formula ticked cause a change to the display of a text string so that special characters alter the string format.

Character Modification Action	Key Character
Subscript	*
Superscript start	<
Superscript end	>
Colour Change	|
Colour Reset	#
Underline next character	_
Bold next character	~
Bold and Underline next character	\



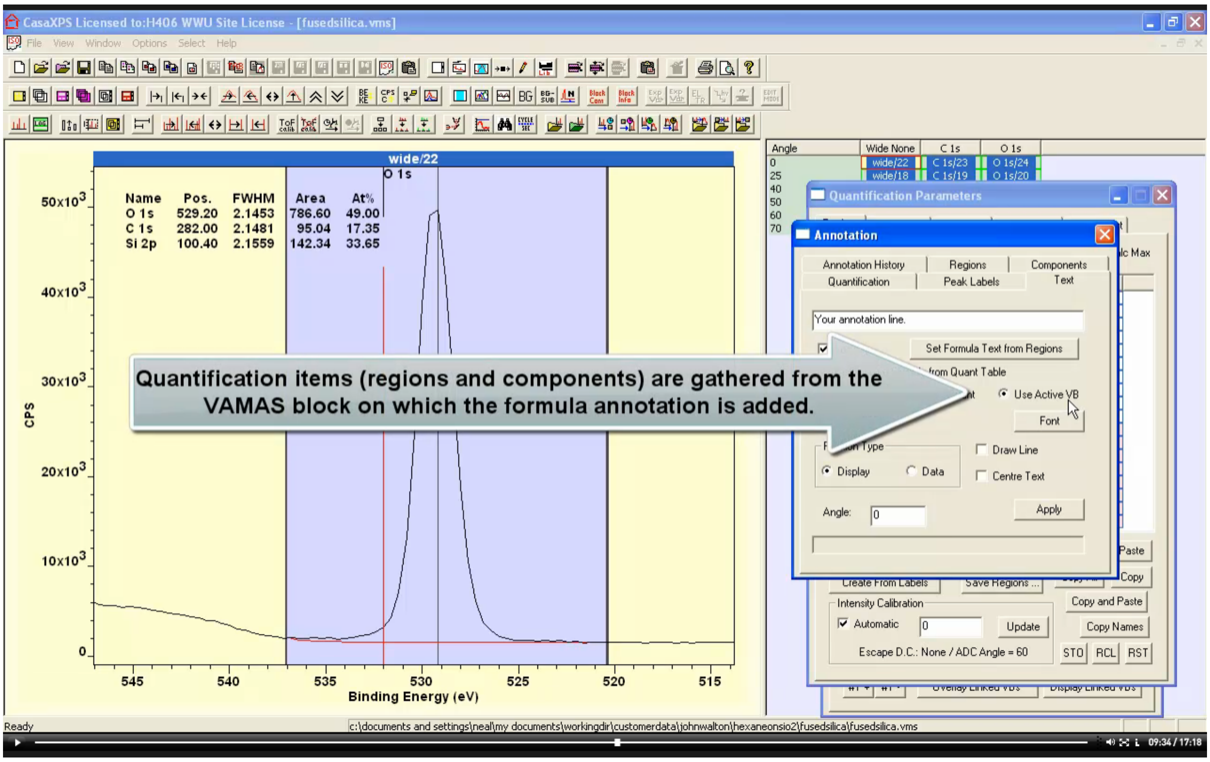
Name	Pos.	FWHM	Area	At%
O 1s	529.20	2.1453	786.60	49.00
C 1s	282.00	2.1481	95.04	17.35
Si 2p	100.40	2.1559	142.34	33.65

A "live" table means the values displayed by the formula string are updated each time regions are modified.

Your annotation line.

☑ Formula
☑ Display Live Formula from Quant Table
○ Use Regions ○ Use Quant ● Use Active VB
☐ Vertical Text
Position Type: ● Display ○ Data
☐ Draw Line
☐ Centre Text
Angle: 0

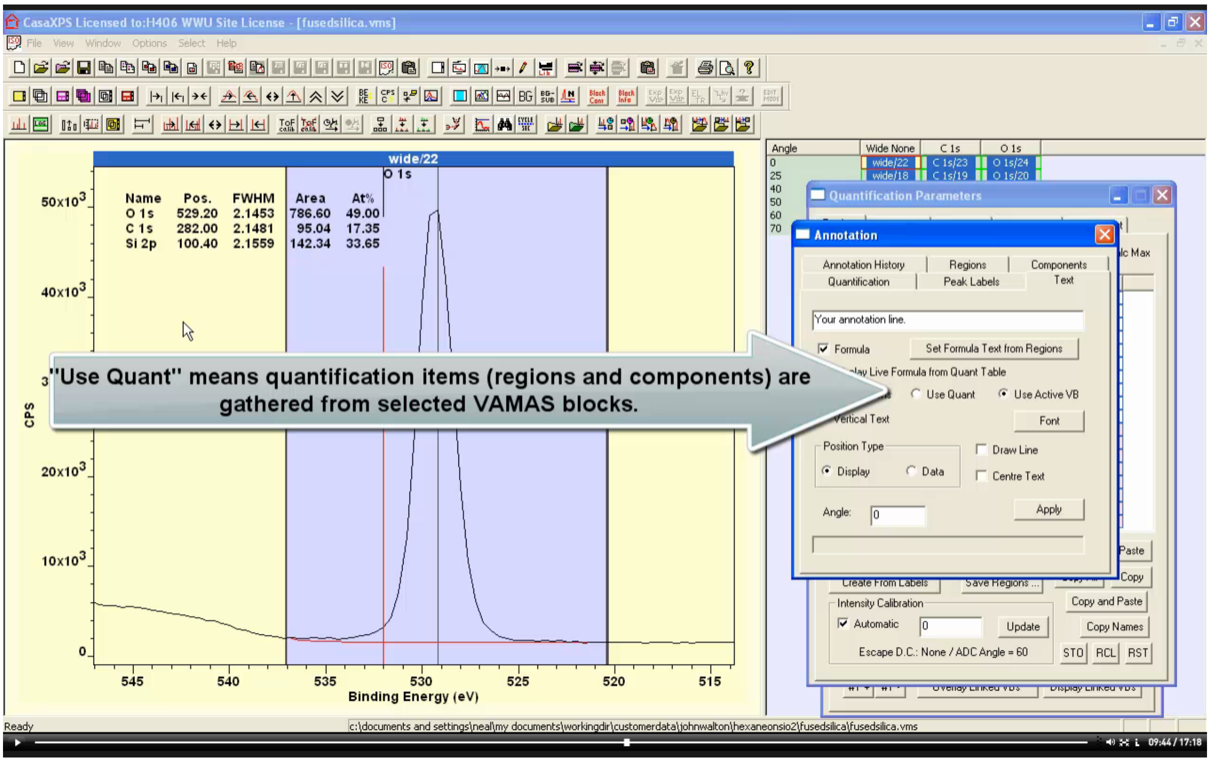
Formatting of elemental symbols is extended by the option labelled Display Live Formula from Quant Table. When active the annotation displayed over data is generated automatically from information gathered from quantification results.



Name	Pos.	FWHM	Area	At%
O 1s	529.20	2.1453	786.60	49.00
C 1s	282.00	2.1481	95.04	17.35
Si 2p	100.40	2.1559	142.34	33.65

Quantification items (regions and components) are gathered from the VAMAS block on which the formula annotation is added.

The most general form of quantification results derives from the selection made for VAMAS blocks in the right hand pane. Regions and components in a peak model are combined to create quantification tables. Both the Quantification Parameters dialog window Report Spec property page and the Annotation dialog window Quantification property page display tabulated results based on selected VAMAS blocks in the right hand pane. There is however an option on the Annotation dialog window Text property page that allows quantification from only the active VAMAS block in the active display tile. The radio button labelled Use Active VB enables gathering of quantification results based on the Active VAMAS block displayed in the active display tile.



"Use Quant" means quantification items (regions and components) are gathered from selected VAMAS blocks.

Name	Pos.	FWHM	Area	At%
O 1s	529.20	2.1453	786.60	49.00
C 1s	282.00	2.1481	95.04	17.35
Si 2p	100.40	2.1559	142.34	33.65

Your annotation line.

☑ Formula

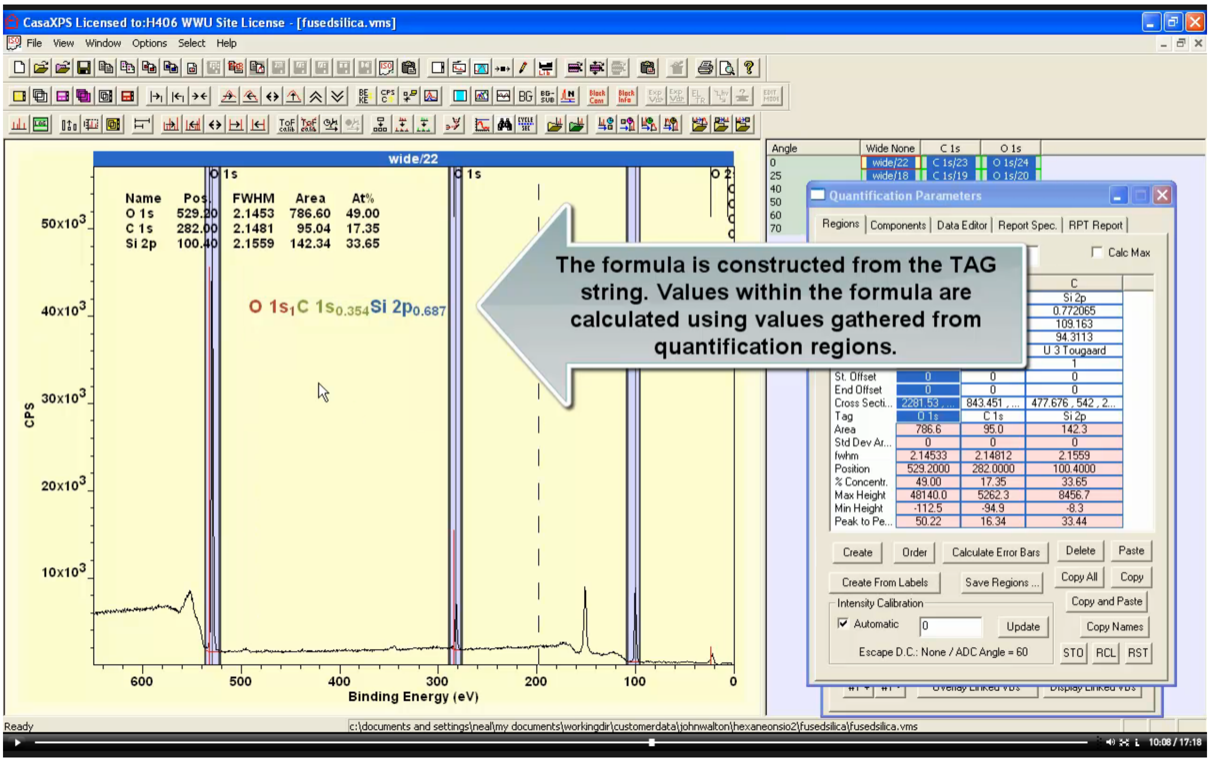
○ Use Quant ● Use Active VB

Position Type: ● Display ○ Data

☐ Draw Line

☐ Centre Text

Angle: 0



The formula is constructed from the TAG string. Values within the formula are calculated using values gathered from quantification regions.

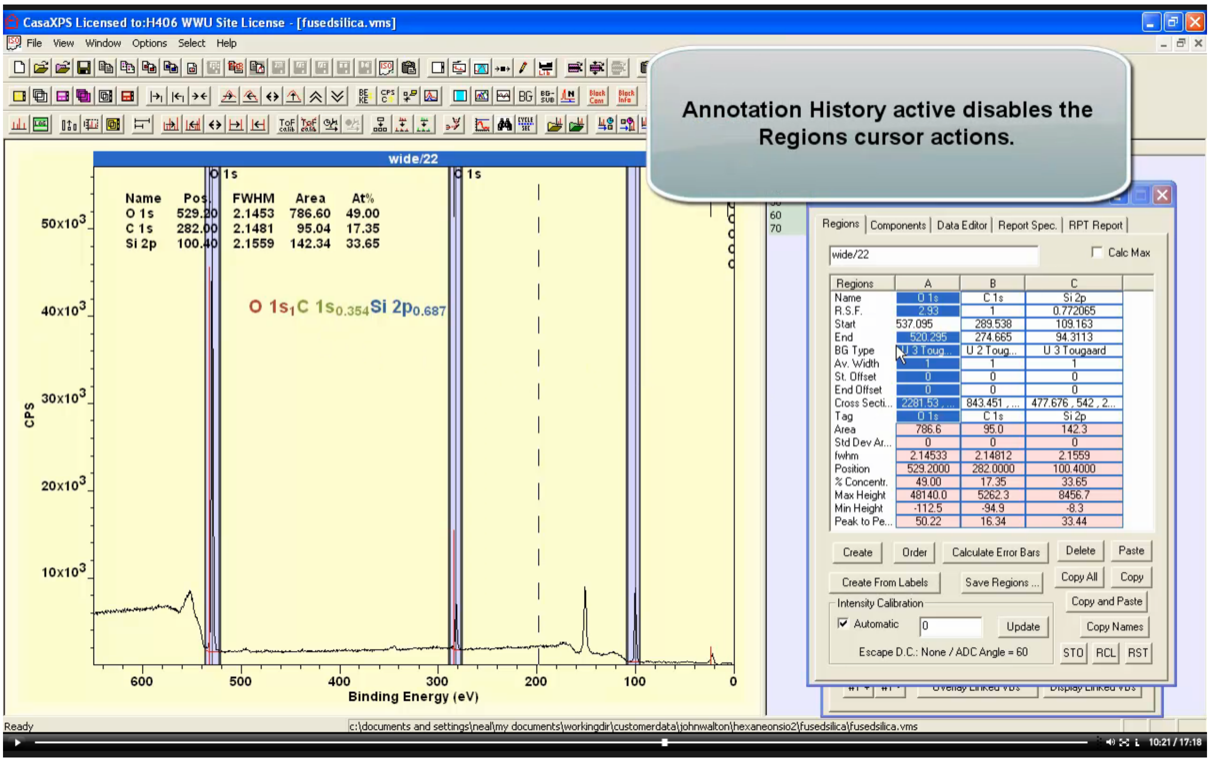
$O\ 1s_{1}C\ 1s_{0.354}Si\ 2p_{0.687}$

			C
			Si 2p
			0.772065
			109.163
			94.3113
			U 3 Tougaard
			1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	2281.53 , ...	843.451 , ...	477.676 , 542 , 2...
Tag	O 1s	C 1s	Si 2p
Area	786.6	95.0	142.3
Std Dev Ar...	0	0	0
fwhm	2.14533	2.14812	2.1559
Position	529.2000	282.0000	100.4000
% Concentr.	49.00	17.35	33.65
Max Height	48140.0	5262.3	8456.7
Min Height	-112.5	-94.9	-8.3
Peak to Pe...	50.22	16.34	33.44

Intensity Calibration: ☑ Automatic 0

Escape D.C.: None / ADC Angle = 60

Text strings used to by formula based annotation text are the strings entered in the TAG fields for regions. TAG string and the use of * character allow changes to the order and numerical values associated with labels entered into the TAG field for each region.



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Annotation History active disables the Regions cursor actions.

Name	Pos	FWHM	Area	At%
O 1s	529.20	2.1453	786.60	49.00
C 1s	282.00	2.1481	95.04	17.35
Si 2p	100.40	2.1559	142.34	33.65

O 1s$_1$C 1s$_{0.354}$Si 2p$_{0.687}$

wide/22

Regions	A	B	C
Name	O 1s	C 1s	Si 2p
R.S.F.	2.93	1	0.772065
Start	537.095	289.538	109.163
End	520.295	274.665	94.3113
BG Type	U 3 Toug...	U 2 Toug...	U 3 Tougaard
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	2281.53 , ...	843.451 , ...	477.676 , 542 , 2...
Tag	O 1s	C 1s	Si 2p
Area	786.6	95.0	142.3
Std Dev Ar...	0	0	0
fwhm	2.14533	2.14812	2.1559
Position	529.2000	282.0000	100.4000
% Concentr.	49.00	17.35	33.65
Max Height	48140.0	5262.3	8456.7
Min Height	-112.5	-94.9	-8.3
Peak to Pe...	50.22	16.34	33.44

☐ Calc Max

Intensity Calibration ☑ Automatic 0

Escape D.C.: None / ADC Angle = 60

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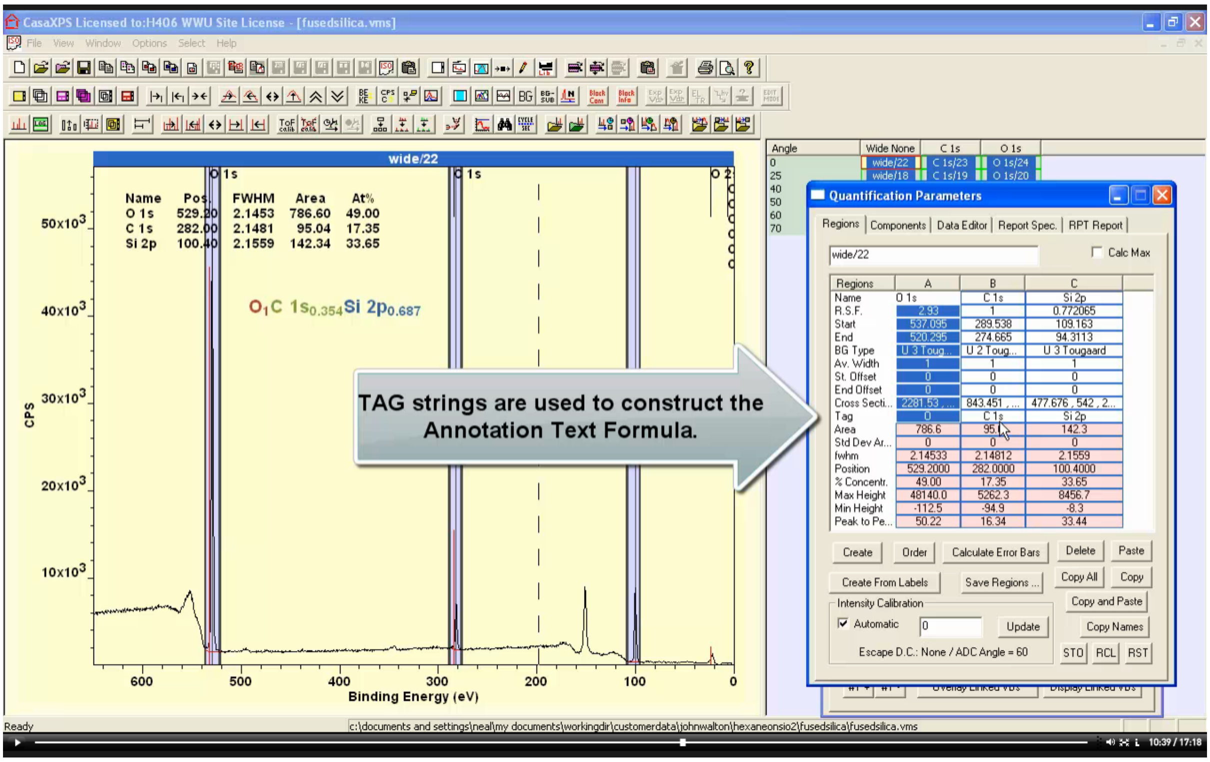

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Name	Pos	FWHM	Area	At%
O 1s	529.20	2.1453	786.60	49.00
C 1s	282.00	2.1481	95.04	17.35
Si 2p	100.40	2.1559	142.34	33.65

O$_1$C 1s$_{0.354}$Si 2p$_{0.687}$

TAG strings are used to construct the Annotation Text Formula.

Angle	Wide None	C 1s	O 1s
0	wide/22	C 1s/23	O 1s/24
25	wide/18	C 1s/19	O 1s/20
40			
50			
60			
70			

Quantification Parameters

wide/22

Regions	A	B	C
Name	O 1s	C 1s	Si 2p
R.S.F.	2.93	1	0.772065
Start	537.095	289.538	109.163
End	520.295	274.665	94.3113
BG Type	U 3 Toug...	U 2 Toug...	U 3 Tougaard
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	2281.53 , ...	843.451 , ...	477.676 , 542 , 2...
Tag	O	C 1s	Si 2p
Area	786.6	95.0	142.3
Std Dev Ar...	0	0	0
fwhm	2.14533	2.14812	2.1559
Position	529.2000	282.0000	100.4000
% Concentr.	49.00	17.35	33.65
Max Height	48140.0	5262.3	8456.7
Min Height	-112.5	-94.9	-8.3
Peak to Pe...	50.22	16.34	33.44

☐ Calc Max

Intensity Calibration ☑ Automatic 0

Escape D.C.: None / ADC Angle = 60

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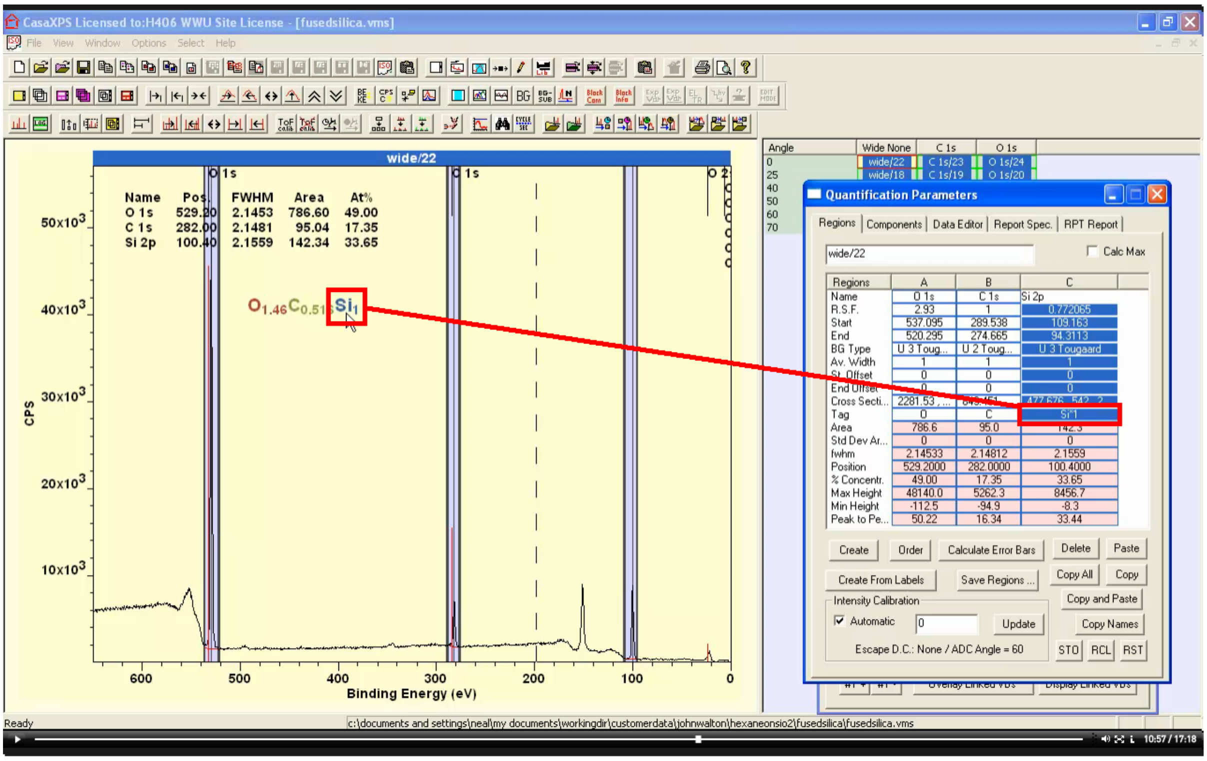
Initially the formula is constructed assuming O appears with a multiplicity of unity, hence the formula is constructed with O_1. If it is preferred to display the formula using the number of silicon atoms is indicated as unity then the TAG field for Si 2p can be adjusted by entering Si * 1.



Name	Pos.	FWHM	Area	At%
O 1s	529.20	2.1453	786.60	49.00
C 1s	282.00	2.1481	95.04	17.35
Si 2p	100.40	2.1559	142.34	33.65

$O_{1.46}C_{0.516}Si_1$

wide/22

☐ Calc Max

Regions	A	B	C
Name	O 1s	C 1s	Si 2p
R.S.F.	2.93	1	0.772065
Start	537.095	289.538	109.163
End	520.295	274.665	94.3113
BG Type	U 3 Toug...	U 2 Toug...	U 3 Tougaard
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	2281.53 , ...	843.451 , ...	477.676 , 542 , 2...
Tag	O	C	Si*1
Area	786.6	95.0	142.3
Std Dev Ar...	0	0	0
fwhm	2.14533	2.14812	2.1559
Position	529.2000	282.0000	100.4000
% Concentr.	49.00	17.35	33.65
Max Height	48140.0	5262.3	8456.7
Min Height	-112.5	-94.9	-8.3
Peak to Pe...	50.22	16.34	33.44

Intensity Calibration

☑ Automatic 0

Escape D.C.: None / ADC Angle = 60

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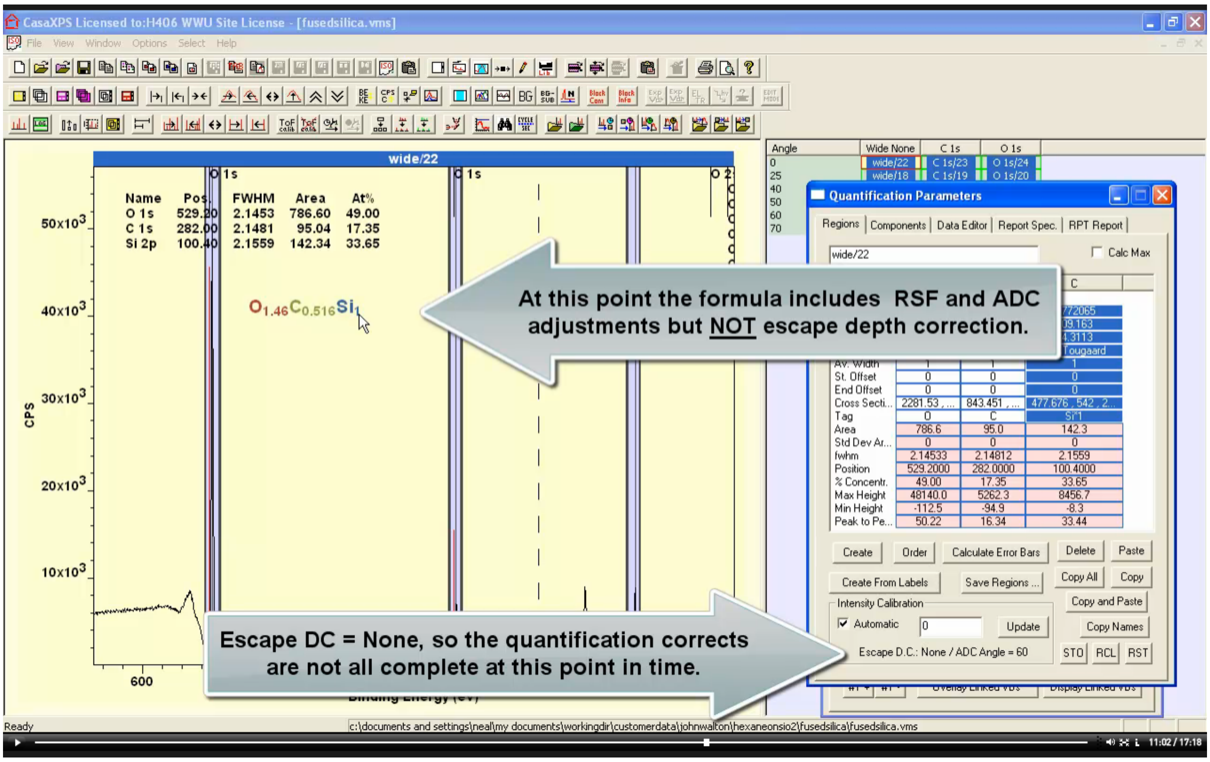
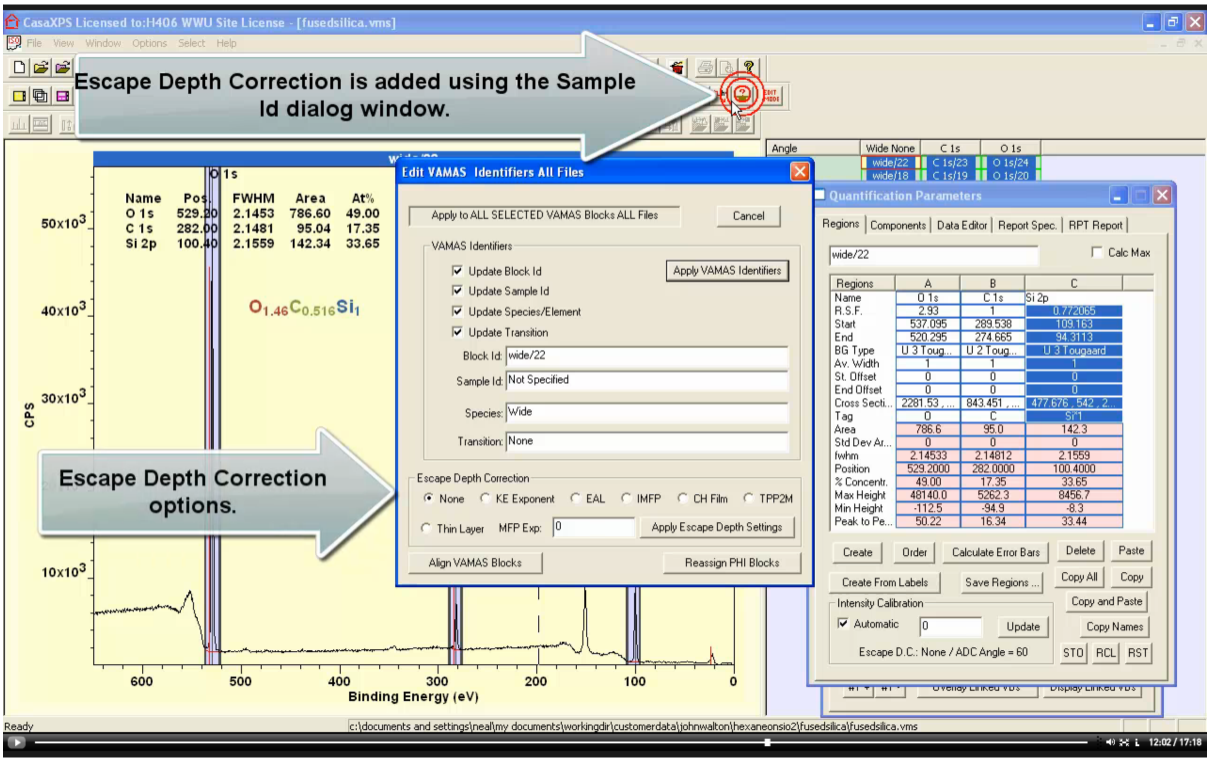


At this point the formula includes RSF and ADC adjustments but NOT escape depth correction.

Escape DC = None, so the quantification corrects are not all complete at this point in time.

As indicated in the Regions property page Intensity Calibration section, the results so far include transmission correction, relative sensitivity corrected for angular distribution but not escape depth correction. Escape depth correction is an important part of quantification and without the correct adjustments for escape depth the correct stoichiometry of two oxygen and one silicon for silica is not returned.



Escape Depth Correction is added using the Sample Id dialog window.

Escape Depth Correction options.

Name	Pos	FWHM	Area	At%
O 1s	529.20	2.1453	786.60	49.00
C 1s	282.00	2.1481	95.04	17.35
Si 2p	100.40	2.1559	142.34	33.65

$O_{1.46}C_{0.516}Si_1$

Edit VAMAS Identifiers All Files

- ☑ Update Block Id
- ☑ Update Sample Id
- ☑ Update Species/Element
- ☑ Update Transition

Block Id: wide/22

Sample Id: Not Specified

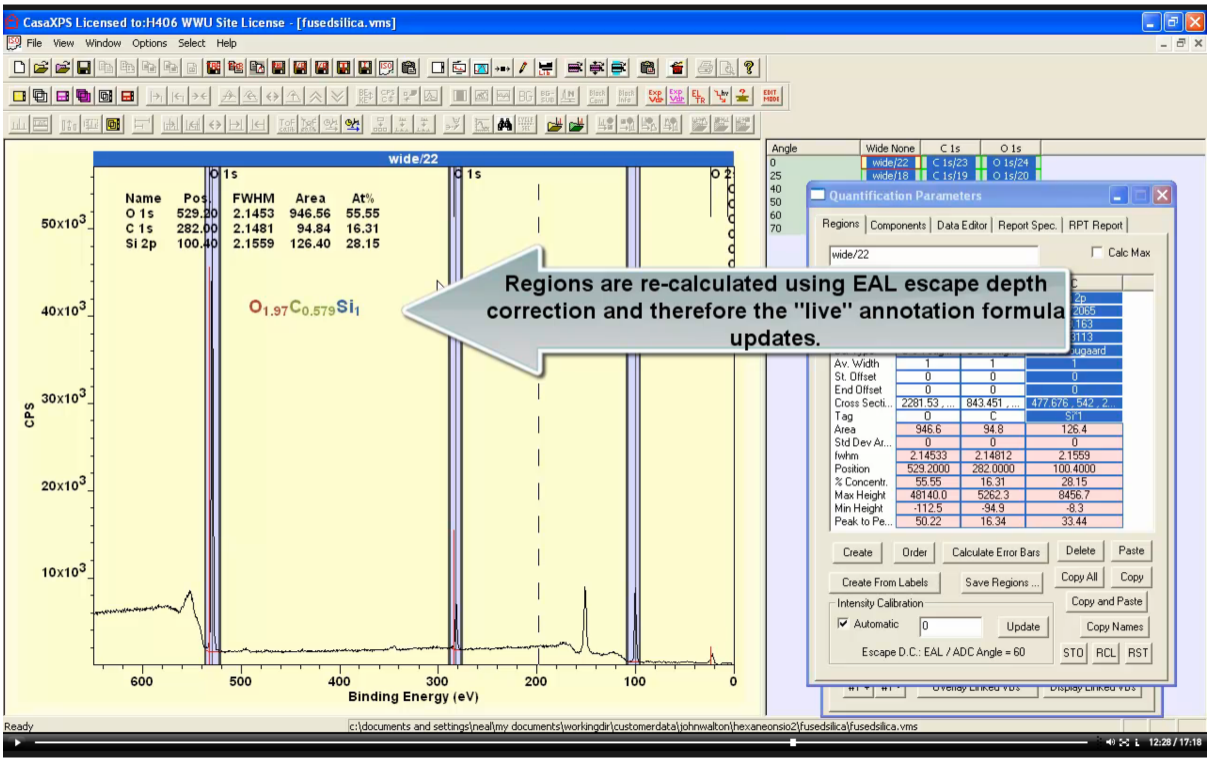
Species: Wide

Transition: None

Escape Depth Correction: ● None ○ KE Exponent ○ EAL ○ IMFP ○ CH Film ○ TPP2M ○ Thin Layer MFP Exp: 0

Regions	A	B	C
Name	O 1s	C 1s	Si 2p
R.S.F.	2.93	1	0.772065
Start	537.095	289.538	109.163
End	520.295	274.665	94.3113
BG Type	U 3 Toug...	U 2 Toug...	U 3 Tougaard
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	2281.53 , ...	843.451 , ...	477.676 , 542 , 2...
Tag	O	C	Si*1
Area	786.6	95.0	142.3
Std Dev Ar...	0	0	0
fwhm	2.14533	2.14812	2.1559
Position	529.2000	282.0000	100.4000
% Concentr.	49.00	17.35	33.65
Max Height	48140.0	5262.3	8456.7
Min Height	-112.5	-94.9	-8.3
Peak to Pe...	50.22	16.34	33.44

Escape depth correction is introduced via selecting VAMAS blocks in the right hand pane then invoking the Edit VAMAS Identifiers dialog window from the toolbar button. For fused silica it will be assumed the material is bulk in nature and therefore EAL (effective attenuation length) correction is appropriate.



Regions are re-calculated using EAL escape depth correction and therefore the "live" annotation formula updates.

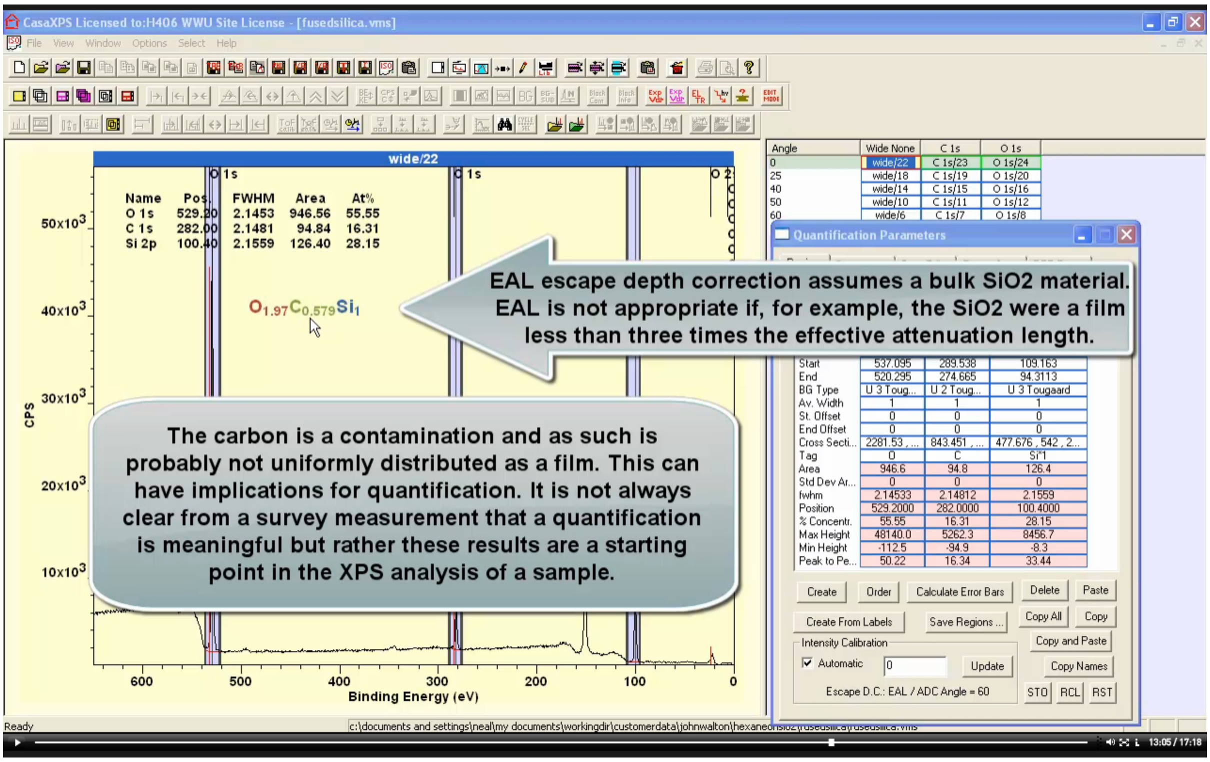
Name	Pos	FWHM	Area	At%
O 1s	529.20	2.1453	946.56	55.55
C 1s	282.00	2.1481	94.84	16.31
Si 2p	100.40	2.1559	126.40	28.15

$O_{1.97}C_{0.579}Si_1$

Regions	A	B	C
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	2281.53 , ...	843.451 , ...	477.676 , 542 , 2...
Tag	O	C	Si*1
Area	946.6	94.8	126.4
Std Dev Ar...	0	0	0
fwhm	2.14533	2.14812	2.1559
Position	529.2000	282.0000	100.4000
% Concentr.	55.55	16.31	28.15
Max Height	48140.0	5262.3	8456.7
Min Height	-112.5	-94.9	-8.3
Peak to Pe...	50.22	16.34	33.44

Escape D.C.: EAL / ADC Angle = 60

Since regions and annotation text are defined using data collected from quantification regions, once the EAL correction is applied both the atomic concentration table and text are updated.



Name	Pos.	FWHM	Area	At%
O 1s	529.20	2.1453	946.56	55.55
C 1s	282.00	2.1481	94.84	16.31
Si 2p	100.40	2.1559	126.40	28.15

$O_{1.97}C_{0.579}Si_1$

EAL escape depth correction assumes a bulk SiO2 material. EAL is not appropriate if, for example, the SiO2 were a film less than three times the effective attenuation length.

The carbon is a contamination and as such is probably not uniformly distributed as a film. This can have implications for quantification. It is not always clear from a survey measurement that a quantification is meaningful but rather these results are a starting point in the XPS analysis of a sample.

Angle	Wide None	C 1s	O 1s
0	wide/22	C 1s/23	O 1s/24
25	wide/18	C 1s/19	O 1s/20
40	wide/14	C 1s/15	O 1s/16
50	wide/10	C 1s/11	O 1s/12
60	wide/6	C 1s/7	O 1s/8

Start	537.095	289.538	109.163
End	520.295	274.665	94.3113
BG Type	U 3 Toug...	U 2 Toug...	U 3 Tougaard
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	2281.53 , ...	843.451 , ...	477.676 , 542 , 2...
Tag	O	C	Si*1
Area	946.6	94.8	126.4
Std Dev Ar...	0	0	0
fwhm	2.14533	2.14812	2.1559
Position	529.2000	282.0000	100.4000
% Concentr.	55.55	16.31	28.15
Max Height	48140.0	5262.3	8456.7
Min Height	-112.5	-94.9	-8.3
Peak to Pe...	50.22	16.34	33.44

Intensity Calibration

☑ Automatic 0

Escape D.C.: EAL / ADC Angle = 60

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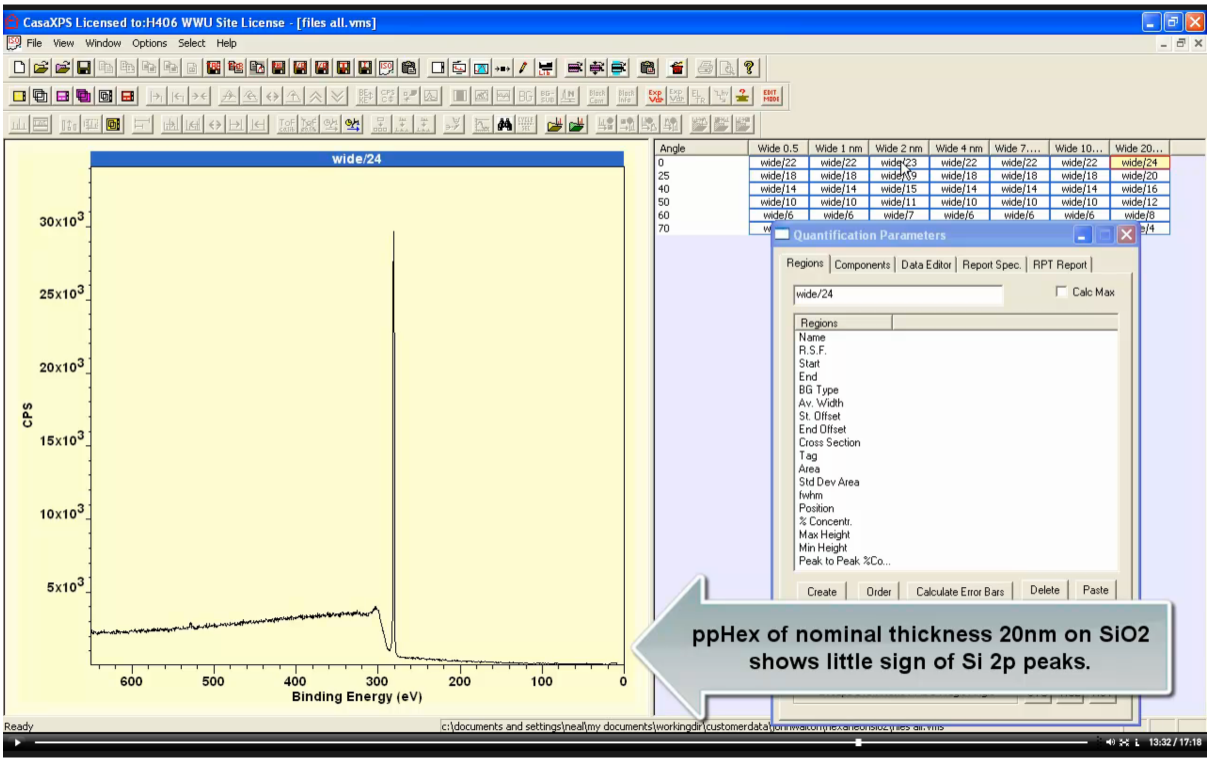
The expected ratio for silicon and oxygen is returned for these data. It should be noted that survey data can be misleading when quantified in isolation. For example the carbon contamination may also include carbon bonded to oxygen so one might expect more oxygen than silicon given the amount of carbon measured by XPS. An alternative argument might be made where it is assumed the contamination by carbon is not uniformly spread over the fused silica but appears as islands of thickness about 10nm. If islands of carbon exist then silicon signal from beneath the contamination would be attenuated less than O 1s signal so one might conceive as scenario where silicon appears more intense than oxygen. It is also possible elemental silicon is involved and this too could shift the composition measure by XPS towards silicon. High energy resolution spectra for Si 2p would remove this possibility.

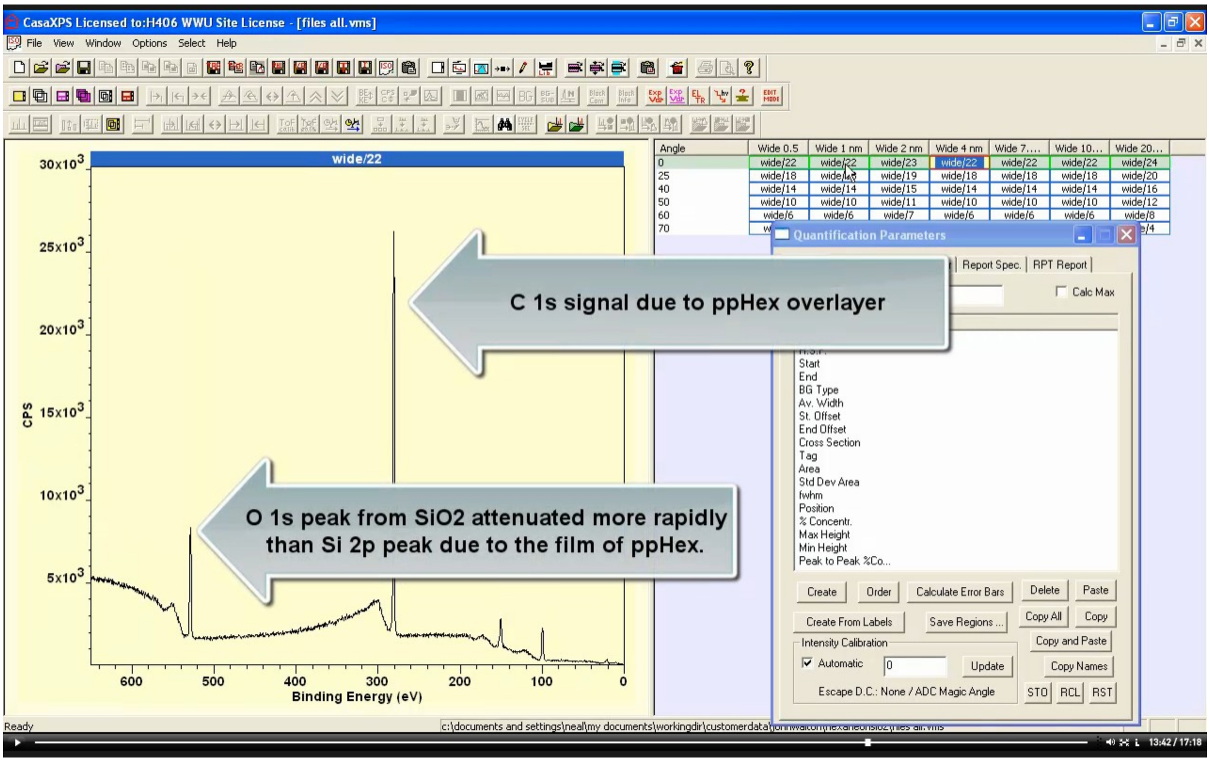
These fused silica data represented a control experiment for a set of samples prepared with films of plasma polymerised hexane (ppHex) on SiO_2. These samples of interest to the paper by Walton et al also provide some insight into the influence of escape depth on general quantification by XPS. By considering how these quantification steps applied to fused silica, when applied to samples with known films alter quantification for a substrate of similar composition to fused silica, it is clear quantification of samples of less well defined origin requires careful consideration.



Angle	Wide 0.5	Wide 1 nm	Wide 2 nm	Wide 4 nm	Wide 7....	Wide 10...	Wide 20...
0	wide/22	wide/22	wide/23	wide/22	wide/22	wide/22	wide/24
25	wide/18	wide/18	wide/19	wide/18	wide/18	wide/18	wide/20
40	wide/14	wide/14	wide/15	wide/14	wide/14	wide/14	wide/16
50	wide/10	wide/10	wide/11	wide/10	wide/10	wide/10	wide/12
60	wide/6	wide/6	wide/7	wide/6	wide/6	wide/6	wide/8
70	w						e/4

ppHex of nominal thickness 20nm on SiO2 shows little sign of Si 2p peaks.

A thick film of ppHex greater than the sampling depth for Si 2p and O 1s the influence of SiO_2 substrate on XPS data is only visible in shapes observed in the inelastic scattered background. That is to say, almost all electrons from Si 2p and O 1s undergo energy loss events therefore these photoemission peaks are absent from the spectrum.

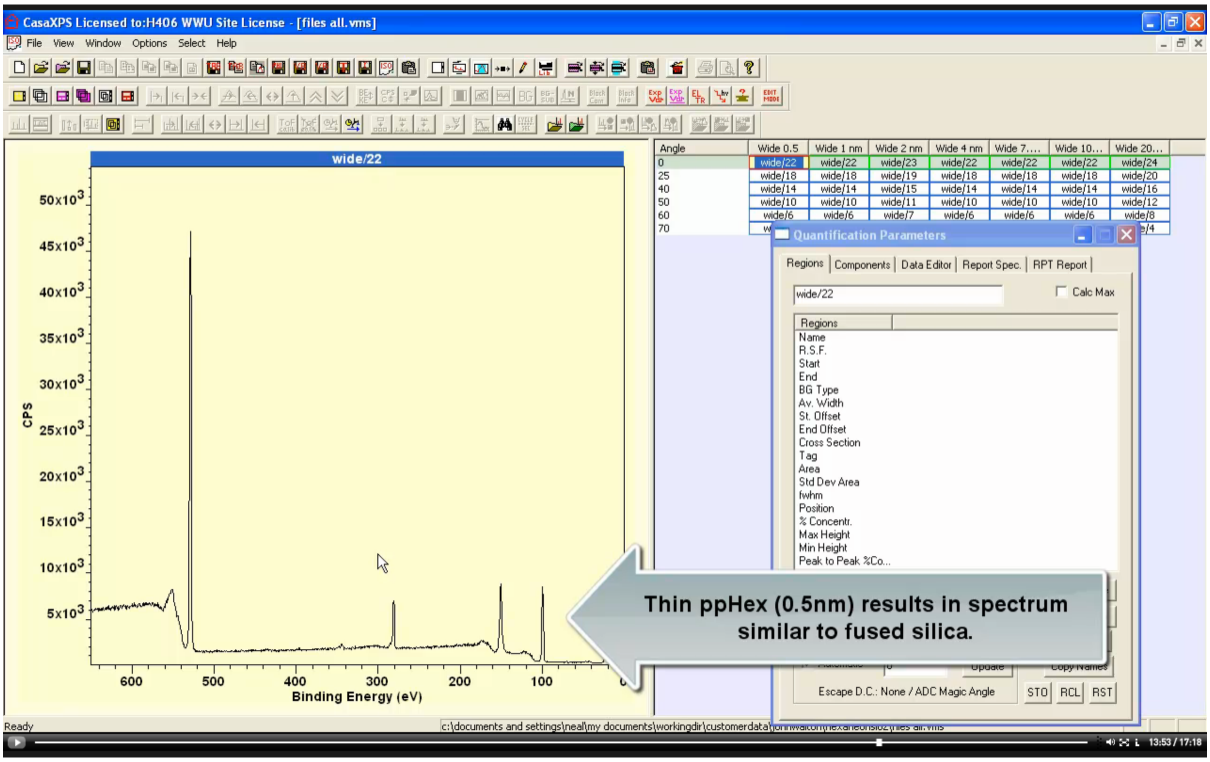


Angle	Wide 0.5	Wide 1 nm	Wide 2 nm	Wide 4 nm	Wide 7....	Wide 10...	Wide 20...
0	wide/22	wide/22	wide/23	wide/22	wide/22	wide/22	wide/24
25	wide/18	wide/18	wide/19	wide/18	wide/18	wide/18	wide/20
40	wide/14	wide/14	wide/15	wide/14	wide/14	wide/14	wide/16
50	wide/10	wide/10	wide/11	wide/10	wide/10	wide/10	wide/12
60	wide/6	wide/6	wide/7	wide/6	wide/6	wide/6	wide/8
70	w						e/4

C 1s signal due to ppHex overlayer

O 1s peak from SiO2 attenuated more rapidly than Si 2p peak due to the film of ppHex.

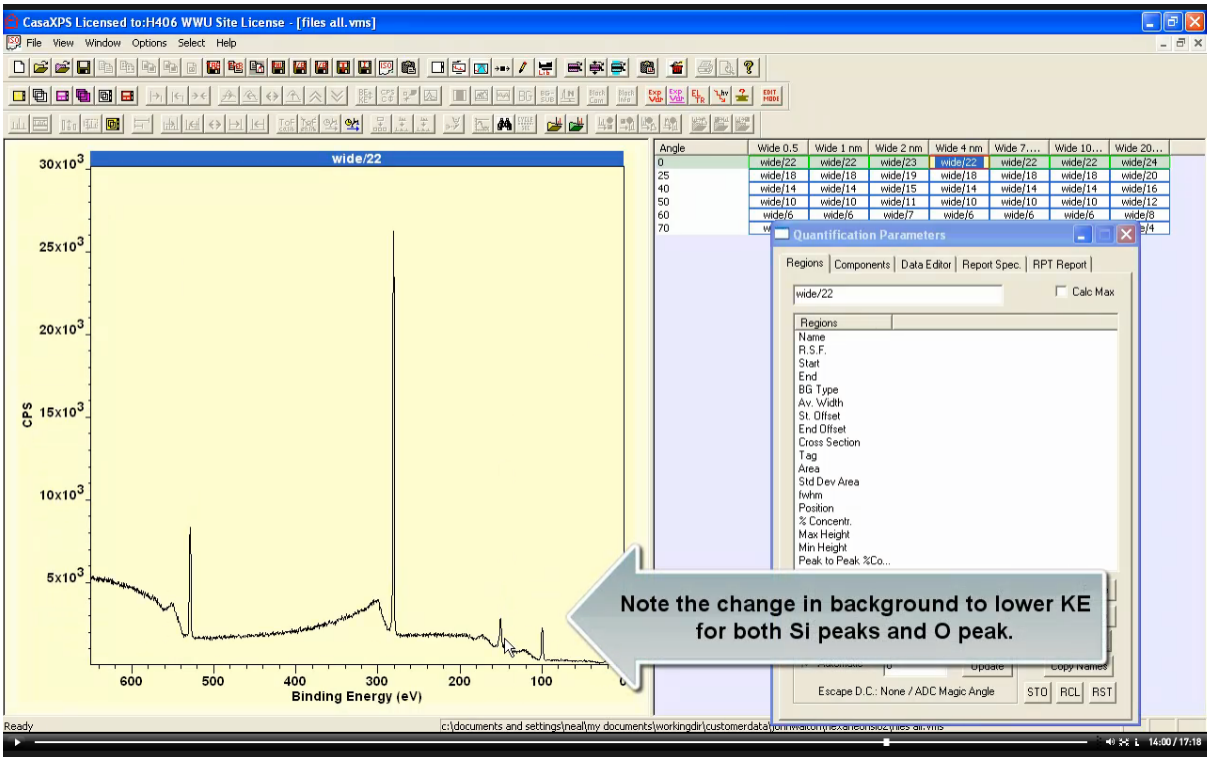
A sample prepared with ppHex depth less than the sampling depth for Si 2p and O 1s electrons, peaks are evident within the spectrum and background shapes indicate an overlayer that does not contain silica.



Angle	Wide 0.5	Wide 1 nm	Wide 2 nm	Wide 4 nm	Wide 7....	Wide 10...	Wide 20...
0	wide/22	wide/22	wide/23	wide/22	wide/22	wide/22	wide/24
25	wide/18	wide/18	wide/19	wide/18	wide/18	wide/18	wide/20
40	wide/14	wide/14	wide/15	wide/14	wide/14	wide/14	wide/16
50	wide/10	wide/10	wide/11	wide/10	wide/10	wide/10	wide/12
60	wide/6	wide/6	wide/7	wide/6	wide/6	wide/6	wide/8
70	w						e/4

Thin ppHex (0.5nm) results in spectrum similar to fused silica.

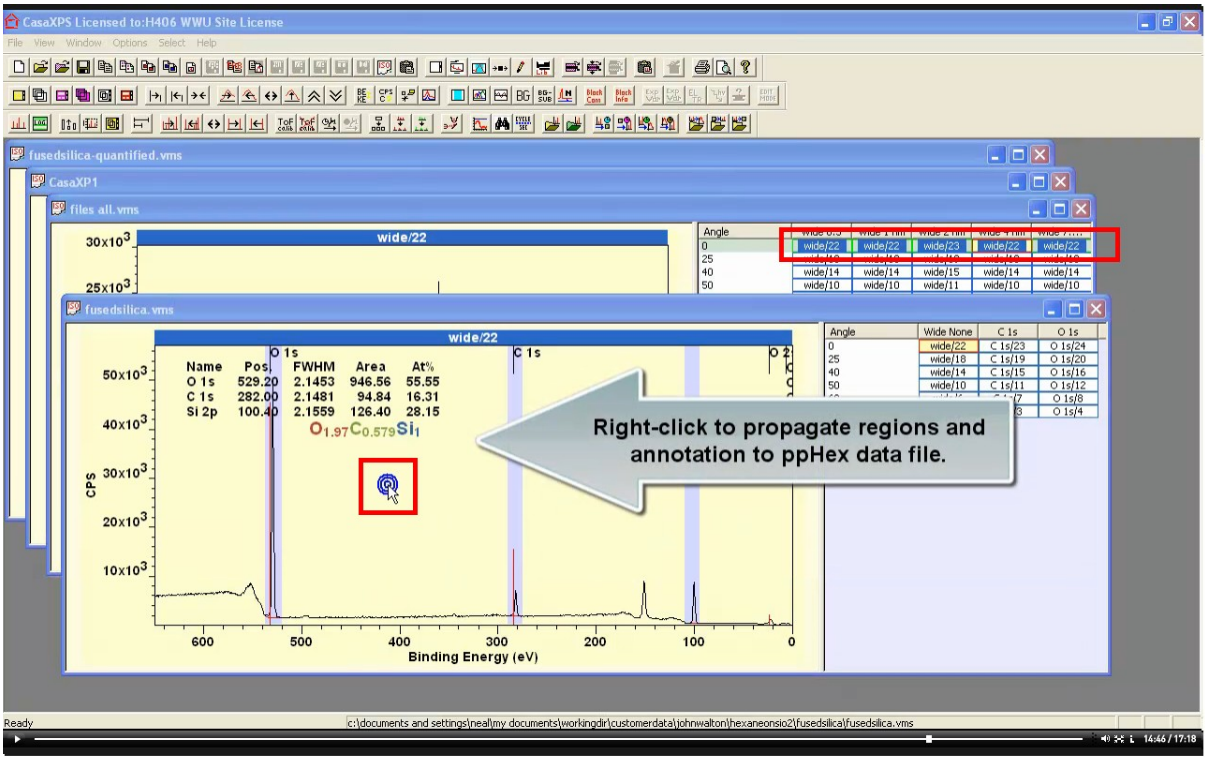
For very thin ppHex on SiO_2 it is difficult by-eye to see the difference from as received fused silica.



Angle	Wide 0.5	Wide 1 nm	Wide 2 nm	Wide 4 nm	Wide 7....	Wide 10...	Wide 20...
0	wide/22	wide/22	wide/23	wide/22	wide/22	wide/22	wide/24
25	wide/18	wide/18	wide/19	wide/18	wide/18	wide/18	wide/20
40	wide/14	wide/14	wide/15	wide/14	wide/14	wide/14	wide/16
50	wide/10	wide/10	wide/11	wide/10	wide/10	wide/10	wide/12
60	wide/6	wide/6	wide/7	wide/6	wide/6	wide/6	wide/8
70	w						e/4

Note the change in background to lower KE for both Si peaks and O peak.

Note how the background to the C 1s overlay of ppHex is very different from background to lower kinetic energy for Si 2p and O 1s photoemission.

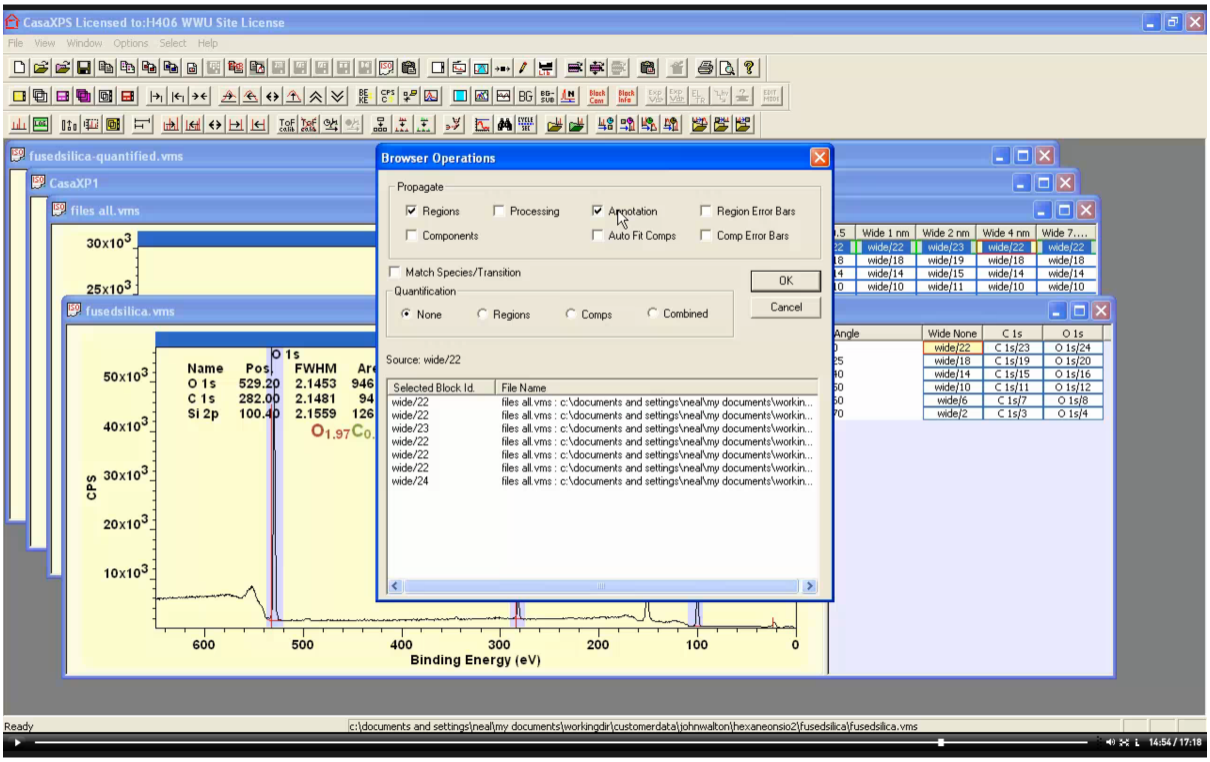


Name	Pos	FWHM	Area	At%
O 1s	529.20	2.1453	946.56	55.55
C 1s	282.00	2.1481	94.84	16.31
Si 2p	100.40	2.1559	126.40	28.15

$O_{1.97}C_{0.579}Si_1$

Right-click to propagate regions and annotation to ppHex data file.

Regions and annotation previously defined for the fused silica VAMAS block are transferred to the ppHex spectra making use of the Browser Operations dialog window.



Browser Operations

Propagate

☑ Regions ☐ Processing ☑ Annotation ☐ Region Error Bars

☐ Components ☐ Auto Fit Comps ☐ Comp Error Bars

☐ Match Species/Transition

Quantification

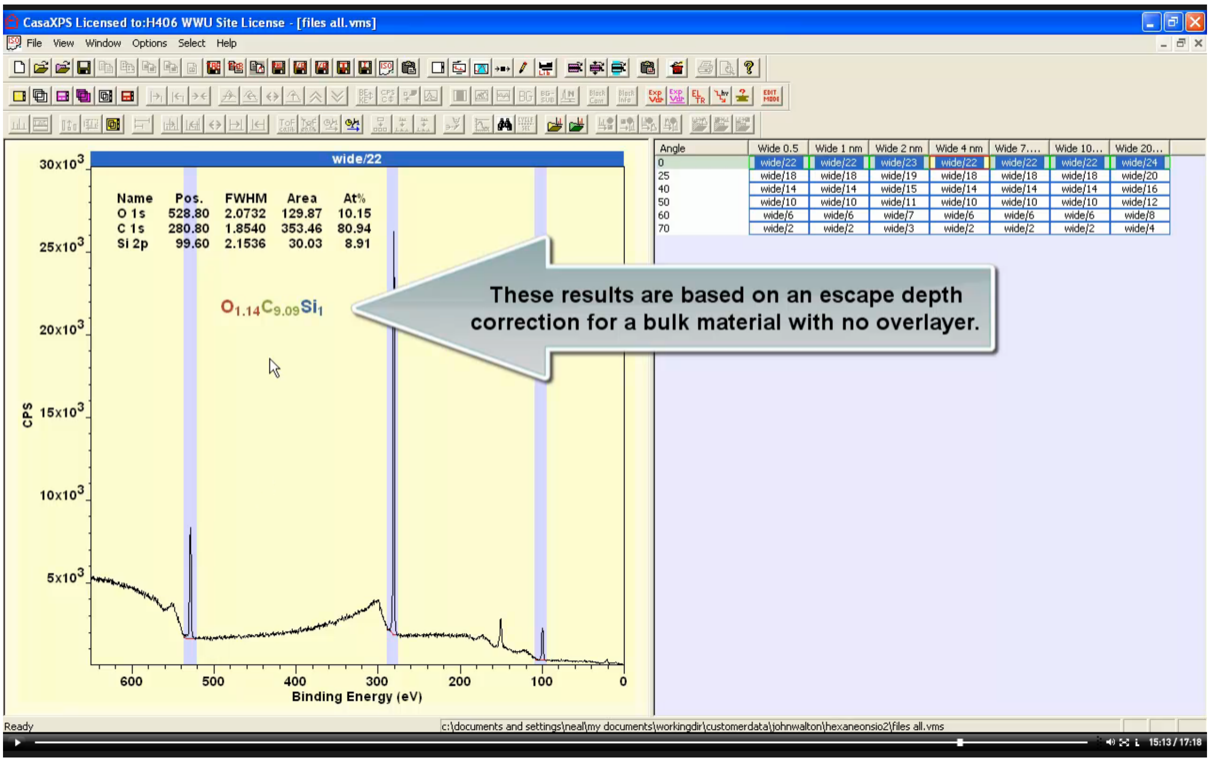
● None ○ Regions ○ Comps ○ Combined

OK Cancel

Source: wide/22

Selected Block Id.	File Name
wide/22	files all.vms : c:\documents and settings\neal\my documents\workin...
wide/22	files all.vms : c:\documents and settings\neal\my documents\workin...
wide/23	files all.vms : c:\documents and settings\neal\my documents\workin...
wide/22	files all.vms : c:\documents and settings\neal\my documents\workin...
wide/22	files all.vms : c:\documents and settings\neal\my documents\workin...
wide/22	files all.vms : c:\documents and settings\neal\my documents\workin...
wide/24	files all.vms : c:\documents and settings\neal\my documents\workin...

VAMAS blocks selected in the right hand pane receive regions and annotation from data displayed in the active tile.



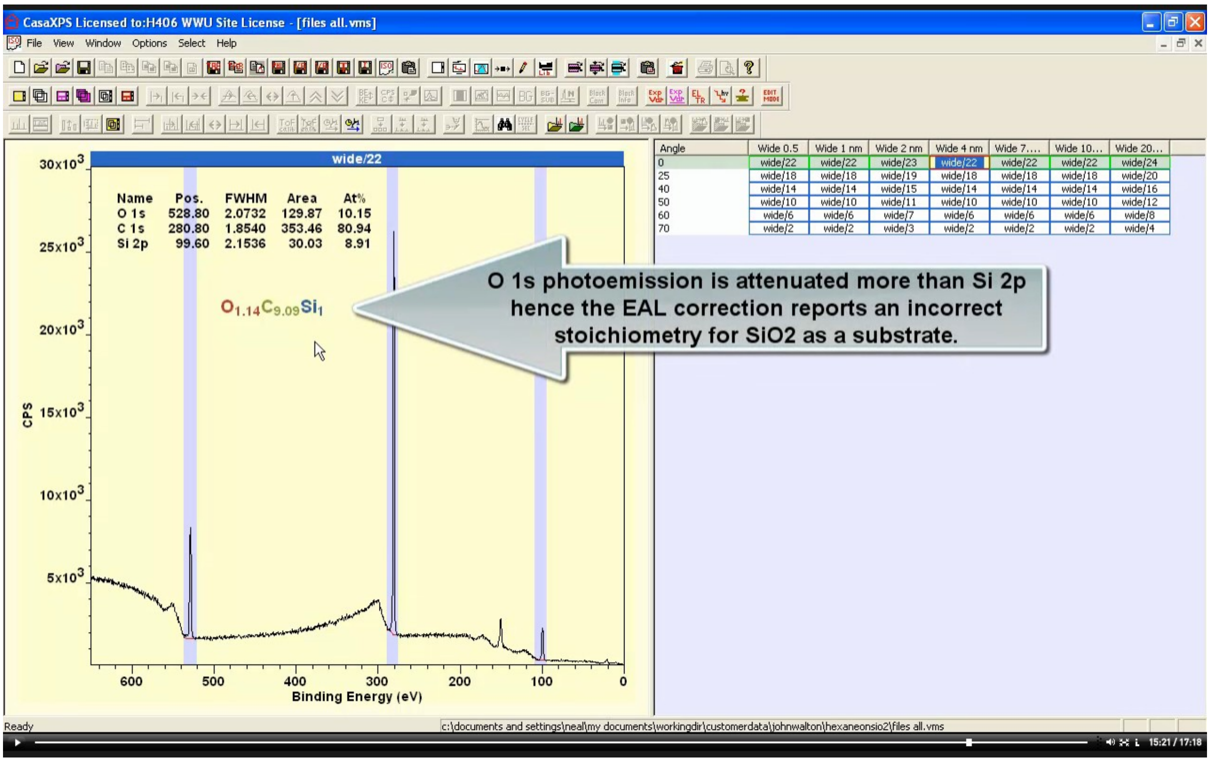
Name	Pos.	FWHM	Area	At%
O 1s	528.80	2.0732	129.87	10.15
C 1s	280.80	1.8540	353.46	80.94
Si 2p	99.60	2.1536	30.03	8.91

$O_{1.14}C_{9.09}Si_{1}$

These results are based on an escape depth correction for a bulk material with no overlayer.

Angle	Wide 0.5	Wide 1 nm	Wide 2 nm	Wide 4 nm	Wide 7....	Wide 10...	Wide 20...
0	wide/22	wide/22	wide/23	wide/22	wide/22	wide/22	wide/24
25	wide/18	wide/18	wide/19	wide/18	wide/18	wide/18	wide/20
40	wide/14	wide/14	wide/15	wide/14	wide/14	wide/14	wide/16
50	wide/10	wide/10	wide/11	wide/10	wide/10	wide/10	wide/12
60	wide/6	wide/6	wide/7	wide/6	wide/6	wide/6	wide/8
70	wide/2	wide/2	wide/3	wide/2	wide/2	wide/2	wide/4

Quantification propagated from fused silica includes all the intensity corrections used to quantify fused silica. Therefore these ppHex samples are quantified making an assumption that is false, namely, the samples are homogeneous in lateral and depth distribution.



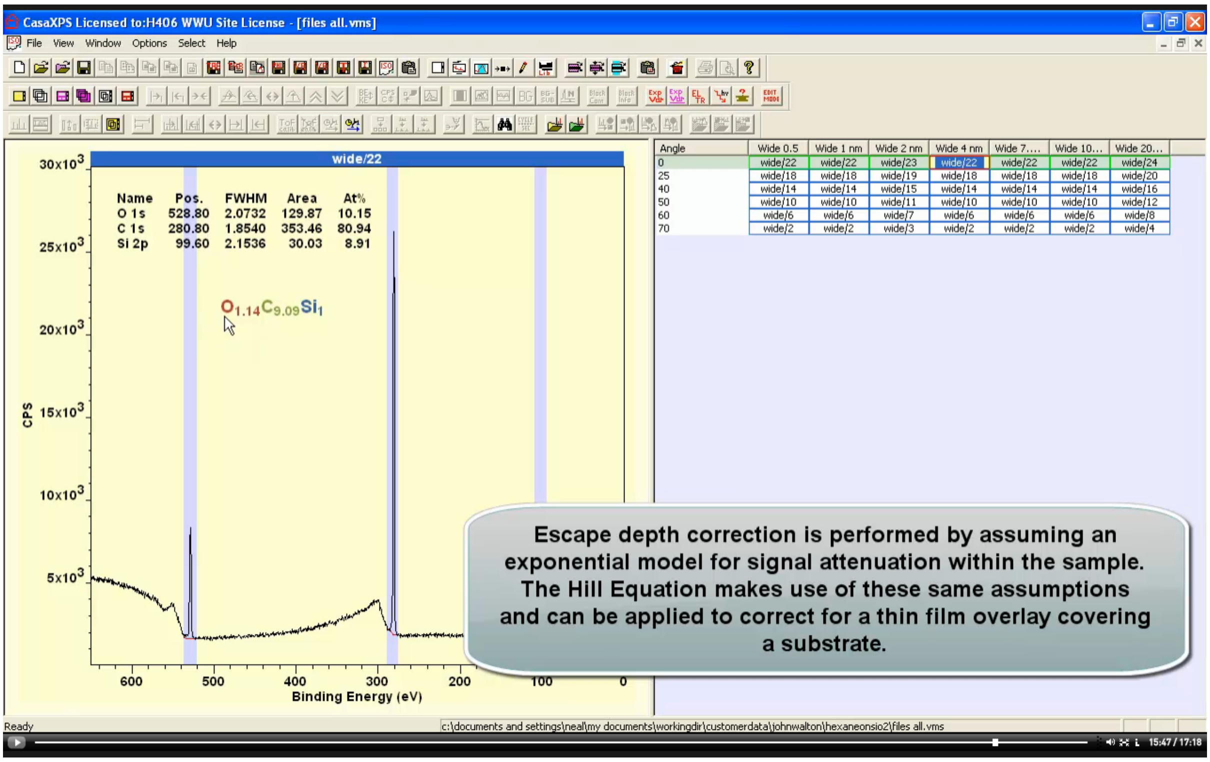
Name	Pos.	FWHM	Area	At%
O 1s	528.80	2.0732	129.87	10.15
C 1s	280.80	1.8540	353.46	80.94
Si 2p	99.60	2.1536	30.03	8.91

$O_{1.14}C_{9.09}Si_{1}$

O 1s photoemission is attenuated more than Si 2p hence the EAL correction reports an incorrect stoichiometry for SiO2 as a substrate.

Angle	Wide 0.5	Wide 1 nm	Wide 2 nm	Wide 4 nm	Wide 7....	Wide 10...	Wide 20...
0	wide/22	wide/22	wide/23	wide/22	wide/22	wide/22	wide/24
25	wide/18	wide/18	wide/19	wide/18	wide/18	wide/18	wide/20
40	wide/14	wide/14	wide/15	wide/14	wide/14	wide/14	wide/16
50	wide/10	wide/10	wide/11	wide/10	wide/10	wide/10	wide/12
60	wide/6	wide/6	wide/7	wide/6	wide/6	wide/6	wide/8
70	wide/2	wide/2	wide/3	wide/2	wide/2	wide/2	wide/4

Since these ppHex samples are layers of ppHex on silicon dioxide when the ratio of oxygen to silicon is reported by the annotation the expected ratio for silicon and oxygen is not achieved.



Name	Pos.	FWHM	Area	At%
O 1s	528.80	2.0732	129.87	10.15
C 1s	280.80	1.8540	353.46	80.94
Si 2p	99.60	2.1536	30.03	8.91

$O_{1.14}C_{9.09}Si_1$

Angle	Wide 0.5	Wide 1 nm	Wide 2 nm	Wide 4 nm	Wide 7….	Wide 10…	Wide 20…
0	wide/22	wide/22	wide/23	wide/22	wide/22	wide/22	wide/24
25	wide/18	wide/18	wide/19	wide/18	wide/18	wide/18	wide/20
40	wide/14	wide/14	wide/15	wide/14	wide/14	wide/14	wide/16
50	wide/10	wide/10	wide/11	wide/10	wide/10	wide/10	wide/12
60	wide/6	wide/6	wide/7	wide/6	wide/6	wide/6	wide/8
70	wide/2	wide/2	wide/3	wide/2	wide/2	wide/2	wide/4

Escape depth correction is performed by assuming an exponential model for signal attenuation within the sample. The Hill Equation makes use of these same assumptions and can be applied to correct for a thin film overlay covering a substrate.

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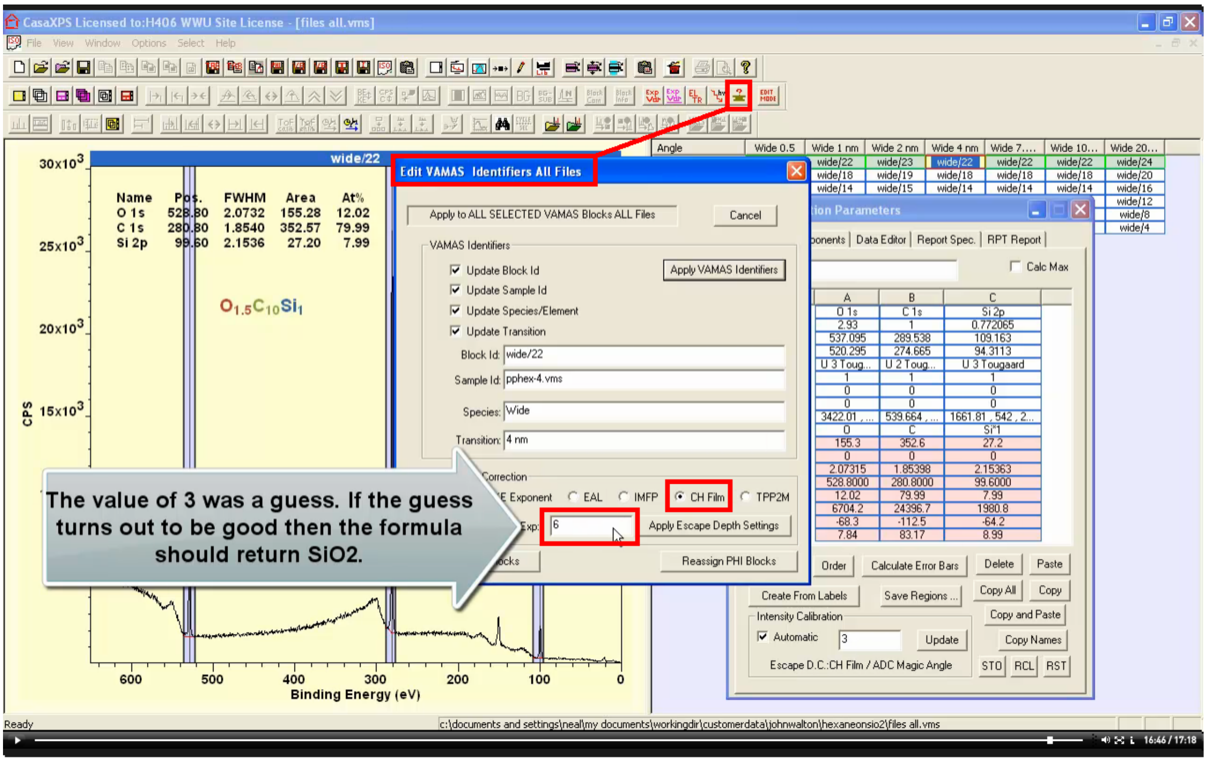
There is an option for correcting a substrate signal for an overlayer. The overlayer ppHex is a CH film so correcting signal from the SiO_2 substrate provides a measure for the film thickness of ppHex.



Name	Pos.	FWHM	Area	At%
O 1s	528.80	2.0732	155.28	12.02
C 1s	280.80	1.8540	352.57	79.99
Si 2p	99.60	2.1536	27.20	7.99

$O_{1.5}C_{10}Si_1$

Edit VAMAS Identifiers All Files

Apply to ALL SELECTED VAMAS Blocks ALL Files

VAMAS Identifiers

- ☑ Update Block Id
- ☑ Update Sample Id
- ☑ Update Species/Element
- ☑ Update Transition

Block Id: wide/22

Sample Id: pphex-4.vms

Species: Wide

Transition: 4 nm

Correction

E Exponent ○ EAL ○ IMFP ● CH Film ○ TPP2M

Exp: 6

A	B	C
O 1s	C 1s	Si 2p
2.93	1	0.772065
537.095	289.538	109.163
520.295	274.665	94.3113
U 3 Toug...	U 2 Toug...	U 3 Tougaard
1	1	1
0	0	0
0	0	0
3422.01 , ...	539.664 , ...	1661.81 , 542 , 2...
O	C	Si*1
155.3	352.6	27.2
0	0	0
2.07315	1.85398	2.15363
528.8000	280.8000	99.6000
12.02	79.99	7.99
6704.2	24396.7	1980.8
-68.3	-112.5	-64.2
7.84	83.17	8.99

☐ Calc Max

Intensity Calibration

☑ Automatic 3

Escape D.C.:CH Film / ADC Magic Angle

The value of 3 was a guess. If the guess turns out to be good then the formula should return SiO2.

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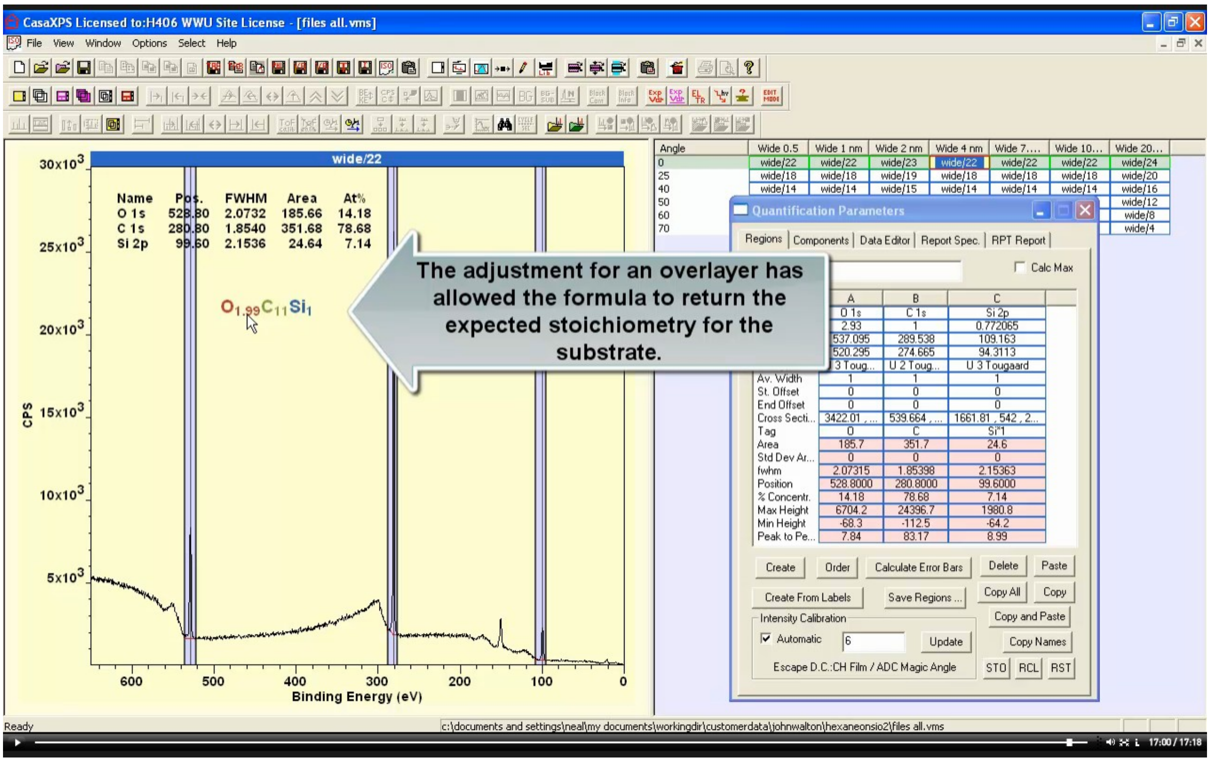
The value entered for the overlayer thickness is based on attenuation assuming an exponential attenuation model. It should be noted that after making such a correction the signal from the overlayer, namely, C 1s is no longer correct as shown in these tables and annotation text.



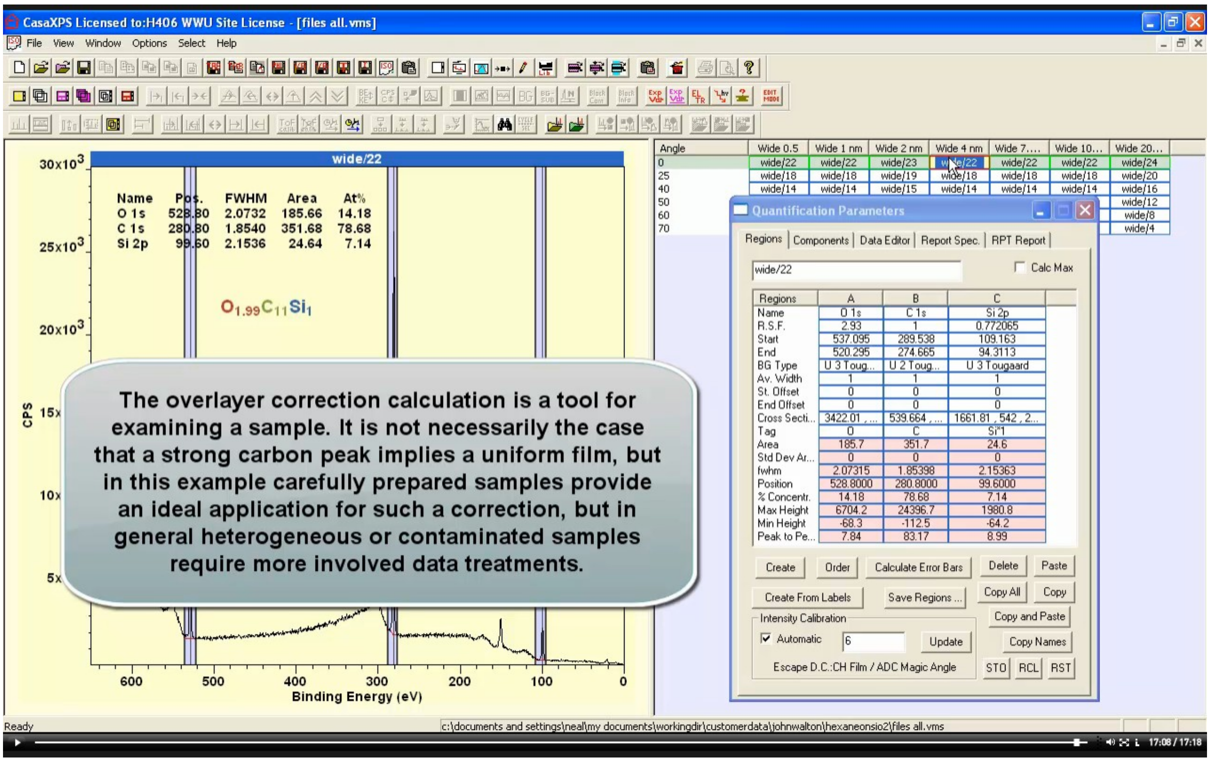
Name	Pos.	FWHM	Area	At%
O 1s	528.80	2.0732	185.66	14.18
C 1s	280.80	1.8540	351.68	78.68
Si 2p	99.60	2.1536	24.64	7.14

$O_{1.99}C_{11}Si_{1}$

The adjustment for an overlayer has allowed the formula to return the expected stoichiometry for the substrate.

Angle	Wide 0.5	Wide 1 nm	Wide 2 nm	Wide 4 nm	Wide 7....	Wide 10...	Wide 20...
0	wide/22	wide/22	wide/23	wide/22	wide/22	wide/22	wide/24
25	wide/18	wide/18	wide/19	wide/18	wide/18	wide/18	wide/20
40	wide/14	wide/14	wide/15	wide/14	wide/14	wide/14	wide/16
50							wide/12
60							wide/8
70							wide/4

	A	B	C
	O 1s	C 1s	Si 2p
	2.93	1	0.772065
	537.095	289.538	109.163
	520.295	274.665	94.3113
	3 Toug...	U 2 Toug...	U 3 Tougaard
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	3422.01 , ...	539.664 , ...	1661.81 , 542 , 2...
Tag	O	C	Si*1
Area	185.7	351.7	24.6
Std Dev Ar...	0	0	0
fwhm	2.07315	1.85398	2.15363
Position	528.8000	280.8000	99.6000
% Concentr.	14.18	78.68	7.14
Max Height	6704.2	24396.7	1980.8
Min Height	-68.3	-112.5	-64.2
Peak to Pe...	7.84	83.17	8.99



Name	Pos.	FWHM	Area	At%
O 1s	528.80	2.0732	185.66	14.18
C 1s	280.80	1.8540	351.68	78.68
Si 2p	99.60	2.1536	24.64	7.14

$O_{1.99}C_{11}Si_{1}$

The overlayer correction calculation is a tool for examining a sample. It is not necessarily the case that a strong carbon peak implies a uniform film, but in this example carefully prepared samples provide an ideal application for such a correction, but in general heterogeneous or contaminated samples require more involved data treatments.

Angle	Wide 0.5	Wide 1 nm	Wide 2 nm	Wide 4 nm	Wide 7....	Wide 10...	Wide 20...
0	wide/22	wide/22	wide/23	wide/22	wide/22	wide/22	wide/24
25	wide/18	wide/18	wide/19	wide/18	wide/18	wide/18	wide/20
40	wide/14	wide/14	wide/15	wide/14	wide/14	wide/14	wide/16
50							wide/12
60							wide/8
70							wide/4

Regions	A	B	C
Name	O 1s	C 1s	Si 2p
R.S.F.	2.93	1	0.772065
Start	537.095	289.538	109.163
End	520.295	274.665	94.3113
BG Type	U 3 Toug...	U 2 Toug...	U 3 Tougaard
Av. Width	1	1	1
St. Offset	0	0	0
End Offset	0	0	0
Cross Secti...	3422.01 , ...	539.664 , ...	1661.81 , 542 , 2...
Tag	O	C	Si*1
Area	185.7	351.7	24.6
Std Dev Ar...	0	0	0
fwhm	2.07315	1.85398	2.15363
Position	528.8000	280.8000	99.6000
% Concentr.	14.18	78.68	7.14
Max Height	6704.2	24396.7	1980.8
Min Height	-68.3	-112.5	-64.2
Peak to Pe...	7.84	83.17	8.99