Sputter Depth Profile Analysis of SiO_2 on Si

Introduction

XPS is a surface sensitive technique. In the case of using X-rays of energy 1486.7 eV (aluminium anode X-ray source), the composition of a sample corresponding to less than 10 nm is available to XPS. However, samples with in-depth distribution beyond 10 nm can also be assessed by XPS provided an ion gun is also available to sputter material from the sample surface.

Sputter depth profiles of a sample are performed by cycling between measurement of sample composition by XPS followed by sputtering the surface with an ion beam. Each sputter cycle removes layers of the sample and alters the sample surface chemistry. Calculating percentage concentration by XPS allows each newly exposed surface to be quantified in terms of elemental, and if appropriate, chemical composition. Plotting the evolution of the sample composition obtained by XPS as the ordinate and the etch time as the abscissa yields a set of curves that provide information about the sample at depths unavailable to a measurement of the sample by XPS alone.

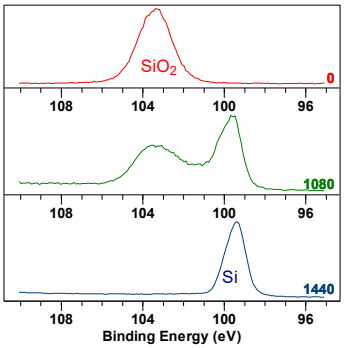

Figure 1. Examples of Si 2p spectra selected from the depth profile spectra to illustrate pure SiO_2 signal, a combination of Si and SiO_2 signal and pure Si signal. The numerical values are the experimental variable, which in the as-received spectra is etch-time in seconds.

The video illustrates features in CasaXPS designed to create (from spectra) a depth profile. The data used in the video were measured on a Thermo Fisher Scientific K Alpha spectrometer. The sample is a silicon wafer with a thick overlayer film of SiO_2. After sputtering for a sufficient duration, the ion beam removes from the analysis area the SiO_2 and creates a surface of elemental silicon. The initial surface is sufficiently thick oxide film of pure SiO_2 that Si 2p spectra are characteristic of bulk SiO_2. However, the etch rate of the ion beam after a period of time uncovers elemental silicon. Since Si and SiO_2 Si 2p photoelectrons are offset in binding energy, the experimental data includes spectra that are characteristic of bulk Si and SiO_2 and varying amounts of thin film SiO_2 on Si which can be separated in terms of intensity into oxide and elemental signal using a peak model (Figure

1). Therefore, despite the simplicity of the sample, the analysis of the profile data set illustrates aspects of data analysis typical of XPS in general. Included in the video is an example of estimating a film thickness using the Hill equation and calibrating the depth-axis of a depth profile using an estimate for the etch rate of SiO_2.

Notes to Accompany the Video

The first step in the analysis of a depth profile experiment is to convert data from the native format of the acquisition system to the ISO 14976 format VAMAS files used by CasaXPS. These data were collected using the Avantage acquisition system, therefore the binary VGD data files of Avantage must be converted to ASCII equivalent AVG format (Figure 2). These AVG ASCII files contain experimental context for the spectra which permits CasaXPS to create a VAMAS file with information necessary for the construction of a depth profile. Further details of how to create AVG files and the methods available in CasaXPS for converting folders of AVG files to VAMAS format is described elsewhere. One of the options used to convert AVG files to VAMAS format is illustrated in the video (Figure 3).

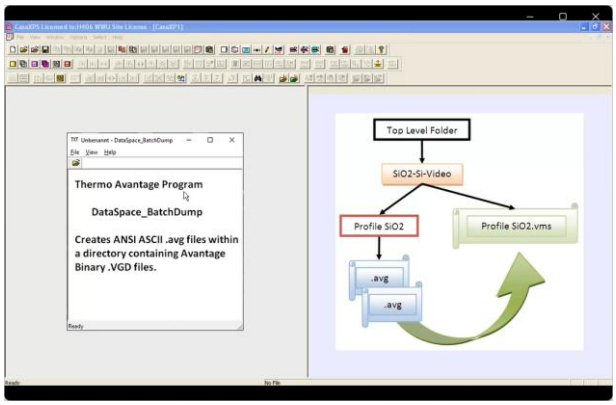

Figure 2. Lefthand Pane: An empty experiment window is used to display BMP image files that name the Avantage program used to convert VGD files to AVG format. Righthand Pane: illustrates the folder structure that contains AVG files and the result of using the conversion filter shown in Figure 3.

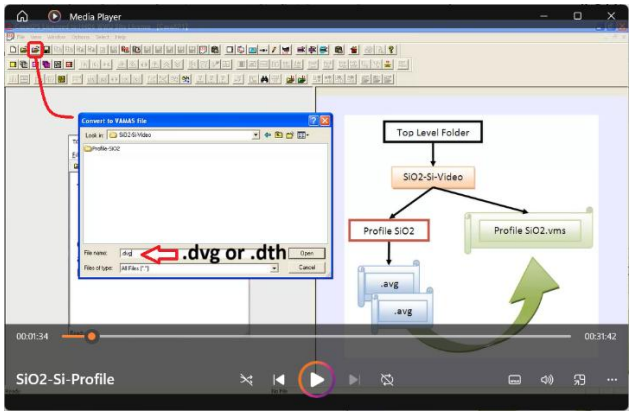

Figure 3. Convert to VAMAS file dialog window used to identify the folder containing AVG files and the use of the ".dvg" conversion filter, the result of which is a new VAMAS file

located at the same level as the folder containing the AVG files. The more recently implemented ".dth" similarly converts folders of AVG files, but is designed to manage the conversion of more complex experiments than the older ".dvg" filter used in the video.

The conversion filter ".dvg" is used in the video to create from the AVG files in the folder with name Profile-SiO2 a VAMAS file (ISO 14976) format used by CasaXPS (Figure 4). The new VAMAS file is assigned the name of the folder and is opened in CasaXPS.

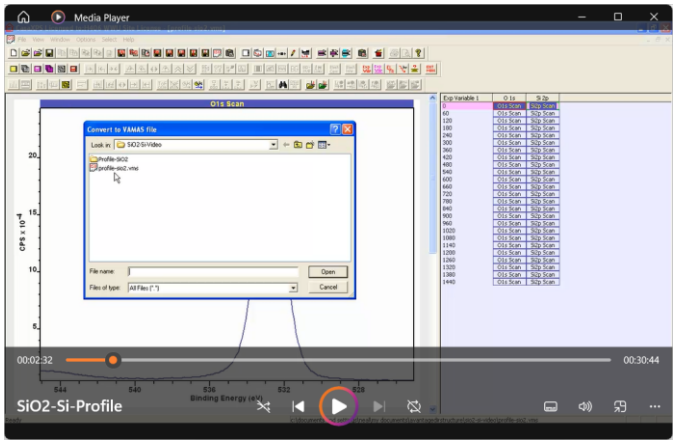

Figure 4. The ".dvg." filter reads the two AVG files corresponding to O 1s and Si 2p spectra within the folder Profile-SiO2 and creates in the same folder as the folder containing Profile-SiO2 the VAMAS file with the name Profile-SiO2.vms.

These two AVG files within the folder Profile-SiO2 represent two sets of narrow scan spectra that correspond to the sputter depth profile XPS cycles. O 1s and Si 2p spectra are listed within these AVG files together with the etch-time information, that is added to the VAMAS blocks created for O 1s and Si 2p as an experimental variable. The experimental variable is used to align in rows VAMAS blocks assigned the same experimental variable (Figure 5). The columns of VAMAS blocks are formed from VAMAS blocks with identical element and transition string fields, hence two columns of spectra appear in the righthand-pane of CasaXPS.

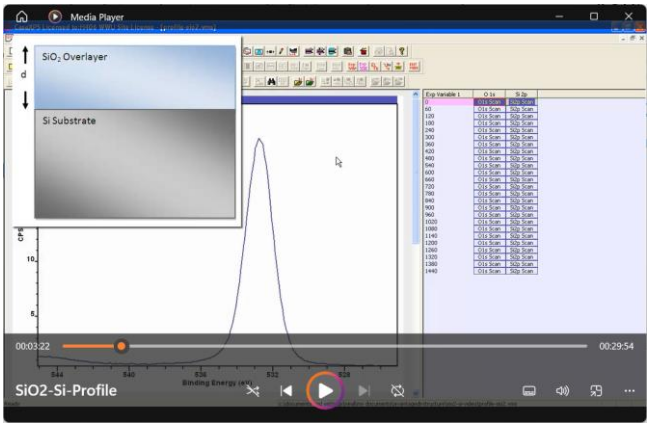

Figure 5. The VAMAS file contains VAMAS blocks, each of which contain spectra, are arranged into rows with common experimental variable (etch-time) and columns using the

identical element/transition VAMAS fields (e.g. element = O, transition = 1s). The idealised model for the sample in-depth composition is illustrated at this point in the video.

The sample consisting of a thick film of SiO_2 on Si is shown in Figure 5 in an idealised form where the film thickness of SiO_2 is d nm. An estimate for the film thickness d nm is the objective for the analysis performed in this video. However, before attempting to calibrate the independent variable of etch-time in seconds to depth in nm, an overview of the depth profile is prepared by creating, so called, quantification regions for the VAMAS blocks containing O 1s and Si 2p spectra. The role of these quantification regions is to specify an energy interval over which a background curve is defined and integration of signal intensity in excess of the background curve provides an estimate for photoelectron peak intensity. These quantification regions are used to assign relative sensitivity (RSF) of photoelectron emission due to photons of a specific energy. The Quantification Parameters dialog window, Regions property page lists quantification regions defined on a VAMAS block. Figure 6 illustrates a quantification region with name O 1s and RSF corresponding to O 1s emission each to 2.93 (Scofield cross-section value for O 1s emission due to scattering by a photon of energy 1486.7 eV). The parameters defined for the quantification region in Figure 6 also include start and end energies that define the limits of integration and the background algorithm used to compute the background curve. The background algorithm is shown in Figure 6 as U 3 Tougaard.

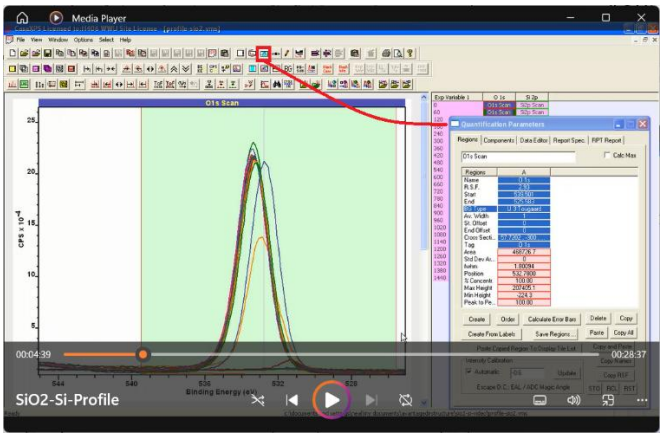

Figure 6. A quantification region is created using the Quantification Parameters dialog window and the Regions property page. When the Create button on the Regions property page is pressed, the active spectrum (first selected VAMAS block of all VAMAS blocks selected when overlaid in the active tile) is updated with a quantification region initially defined with name constructed from the element/transition string (O 1s in this case). If the name matches an entry in the current element library, the RSF is extracted from the element library (2.93) and inserted in the RSF parameter field of the quantification region.

Quantification regions defined on the active VAMAS block in the active tile (the display tile with the title string with a blue background-colour in Figure 6) are propagated from the active VAMAS block to a selection of VAMAS blocks as defined by the righthand-pane.

Placing the cursor over the lefthand-pane active tile before clicking the mouse righthand button invokes the Browser Operations dialog window. Figure 7 illustrates the dialog window used to propagate quantification regions from the active VAMAS block to the selected VAMAS blocks. The example shown in Figure 7 propagates the quantification region defined on the active VAMAS block corresponding to a Si 2p spectrum for which a region has been prepared to the selected Si 2p spectra measured throughout the depth profile experiment. The Browser Operations dialog window includes options to enable or disable different types of information from the active VAMAS block to the selected VAMAS blocks. A list of selected VAMAS blocks is displayed on the Browser Operations dialog window. The example in Figure 7 makes use of the Regions option in the Propagate section of the dialog window only. Hence, only quantification regions are transferred from the active VAMAS block to the selected VAMAS blocks.

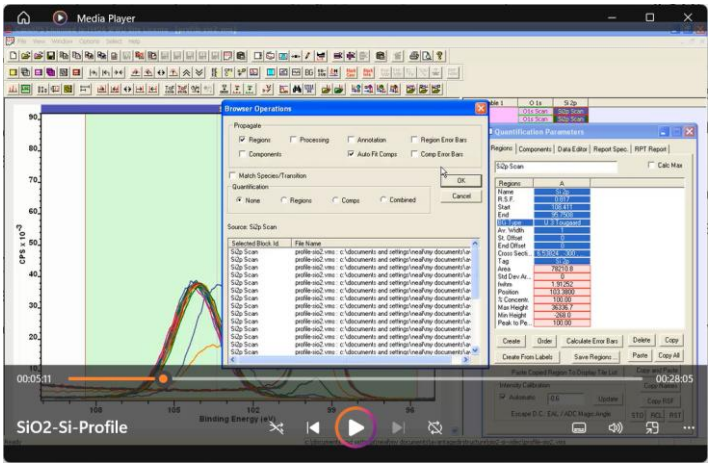

Figure 7. Browser Operations dialog window is used to move quantification regions defined on the active VAMAS block to VAMAS blocks selected in the righthand-pane of the experiment window.

The Quantification Parameters dialog window, Report Spec property page is used to create depth profiles and other profiles from quantification regions, for example. The initial profile created in the video is a tabulation of corrected peak intensities and percentage atomic concentration against etch-time based on quantification regions defined for all O 1s and Si 2p spectra. The progression during the profile from SiO_2 to Si is evidenced by the intensity of O 1s, which only exists in the oxide layer. The inclusion of Si 2p intensity is necessary to make sense of the intensity measured for O 1s. During the course of an experiment, it is possible that photoelectron signal such as O 1s may vary for reasons other than changes in sample chemistry. However, reporting atomic concentration, albeit limited to O 1s and Si 2p, allows the normalisation of O 1s and Si 2p to each other, or rather to the sum of O 1s and Si 2p intensity. Hence, fluctuations in X-ray power, for example, in the course of the profile will likely be accounted for by normalising to the sum of O 1s and Si 2p for each cycle of the profile.

The steps that permit the creation of a depth profile tabulation are illustrated in Figure 8. That is, after quantification regions are defined on the O 1s and Si 2p spectra, selecting the VAMAS blocks in the righthand-pane indicates from which spectra the profile should be created. The selected VAMAS blocks cause a response in the Report Spec Quantification Item Names table (Figure 8), which lists the Name fields gathered from all selected VAMAS blocks with quantification regions defined. The actual definition of the depth profile table derives from the Name/Formula table, which is prepared with a name column and a corresponding column of formulae. The formulae are mathematical expressions in which the quantification item names listed are the variables in the expression that change as the experimental variable changes. The names in the Name/Formula table are used to label in the profile report table the headings to columns of values computed from the formulae. The formulae in Figure 8 are simply the variables that change during the profile, namely, O 1s and Si 2p representing the intensity of each photoelectron peak for each cycle of the depth profile.

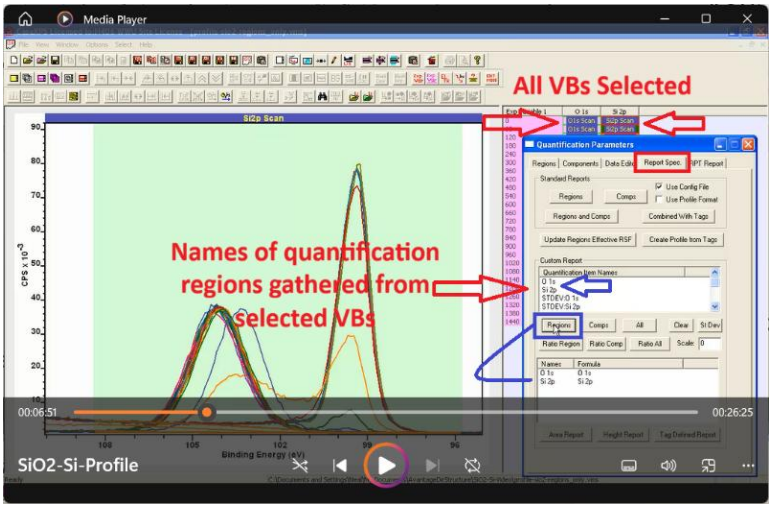

Figure 8. Quantification Parameters dialog window, Report Spec property page. Quantification items refer to quantification regions or components to a peak model. The purpose of quantification items is to name a variable that can be used in the Name/Formula table. These named variables derive from either quantification regions or components. The Quantification Item Names table is populated with the strings entered (Figure 7) in the Names fields for quantification regions (and Components Name field on the Components property page, described below). The Names/Formula table is populated in preparation for the creation of a depth profile tabulation. The Region button marked blue is used to populate the Names/Formula table with the names of quantification regions.

Once the selection of VAMAS blocks has been made using the righthand-pane of the experiment frame and the Name/Formula table prepared as shown in Figure 8, pressing the Area Report button indicated in Figure 9 creates a new window in which the etch-time experimental variable appears as the first column in the table, followed by two columns corresponding to the intensity of photoelectron peaks corrected for elemental and instrumental sensitivity to O 1s and Si 2p emission, and two more columns for percentage

atomic concentration computed from the corrected photoelectron intensity. The units CPS eV for the intensity of O 1s and Si 2p is to inform that the peak areas are integrated using counts per second and integrated with respect to energy. Calculating intensity in CPS eV allows changes in dwell-time and energy step-size used to collect spectra without altering the quantification results.

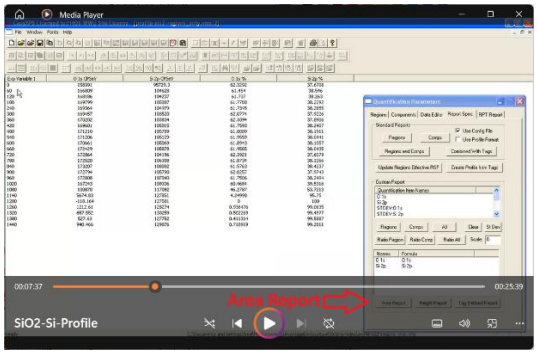

Figure 9. Tabulation of O 1s and Si 2p photoelectron peak intensities corrected for transmission, escape depth and RSFs, followed by percentage atomic concentration columns for these two elements.

The table generated by the Custom Report section of the Quantification Parameters dialog window, Report Spec property page can be converted to a VAMAS file. The first column in the table is the independent variable corresponding to dependent variables computed from spectra that appear in the subsequent columns of the table. Therefore, for each dependent variable a VAMAS block is created in a new VAMAS file, which are separated into rows using an index number for the experimental variable (Figure 10). The top row of VAMAS blocks corresponds to the percentage atomic concentration, while the bottom-row corresponds to the corrected peak intensity for O 1s and Si 2p photoelectron emission.

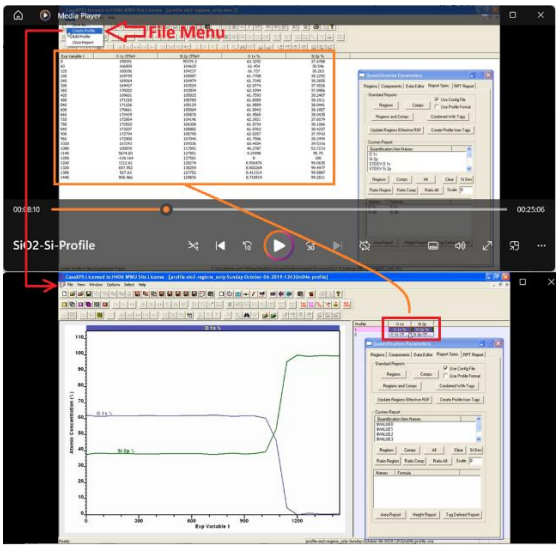

Figure 10. The tabulated depth profile may transfer as tab spaced data through the clipboard to a spreadsheet program, for example, by selecting the Copy toolbar button (Ctrl + C).

Alternatively, the File menu includes a menu item labelled *Create Profile* used to convert the columns in the table into VAMAS blocks in a new VAMAS file.

The analysis in the video that follows is intended to illustrate a scenario in which a peak model is used to estimate the relative proportions of chemical state for oxide and elemental silicon. The excuse for constructing the peak model is a desire to convert etch-time to depth in nanometres and therefore estimate the original thickness of the SiO_2 film on Si substrate. The method used to estimate a film thickness is referred to by the name, Hill Equation. Therefore, the following subsection presents the logic used to derive the Hill equation and may be skipped without loss to the theme of the video.

Calculating Film Thickness using the Hill Equation

A film thickness estimate assumes the emission depth distribution function is exponential in form:

$$\boldsymbol{N(t) = N_0 e^{-\left(\frac{t}{a}\right)}}$$

The parameter t is the depth beneath the surface from which photoemission originates and the constant a is characteristic of the material from which the zero-loss electrons must emerge. The value used for a is the effective attenuation length (EAL). The intensity of electrons emitted by the overlayer I_o of thickness $\boldsymbol{d = t \times cos\theta}$ for a measurement performed at an angle θ to the sample normal is proportional to:

$$\boldsymbol{\frac{1}{a}\int_0^t e^{-\left(\frac{p}{a}\right)} dp = 1 - e^{-\left(\frac{t}{a}\right)}}$$

Similarly, the intensity I_s from the substrate is proportional to:

$$\boldsymbol{\frac{1}{a}\int_t^\infty e^{-\left(\frac{p}{a}\right)} dp = e^{-\left(\frac{t}{a}\right)}}$$

The constant of proportionality in either case is the signal intensity expected for infinitely thick homogenous samples for the overlayer and substrate materials. Thus

$$\boldsymbol{\frac{\left(I_o/I_o^\infty\right)}{\left(I_s/I_s^\infty\right)} = \frac{1 - e^{-\left(\frac{t}{a}\right)}}{e^{-\left(\frac{t}{a}\right)}} = e^{+(t/a)} - 1}$$

On solving for t the equation becomes:

$$\boldsymbol{\frac{t}{a} = ln\left(1 + \frac{\left(I_o/I_o^\infty\right)}{\left(I_s/I_s^\infty\right)}\right)}$$

If the measurement is made at an angle θ to the sample normal, the Hill Equation for an overlayer of thickness d becomes:

Hill Equation:

$$d = a \times \cos\theta \times ln\left(1 + \frac{\left({I_o}/{I_o^{\infty}}\right)}{\left({I_s}/{I_s^{\infty}}\right)}\right)$$

Constructing a Peak Model for Si 2p for use with the Hill Equation

The focus of the video now turns to estimating the sputter rate of SiO_2. Once the sputter rate is obtained, the etch-time can be converted to depth scale that will be, in an ideal world, valid for the overlayer oxide film. The heuristic used to estimate the sputter rate is based on estimating the thickness of the oxide layer at some point during the profile and then estimate the etch-time from the chosen point in the profile to the point in the profile where the overlayer has been completely removed by sputtering. There are some potential problems with this heuristic, so it is not recommended as the best method for estimating the sputter-rate of SiO_2, but the steps involved provide a narrative that guides the lines of discussion that follow.

To estimate the thickness of a film of one material on a different substrate material, the information required involves obtaining an estimate for the CPS eV that would be achieved (for a given operating mode of an instrument) for the overlayer and substrate materials if measured from bulk homogeneous samples of these two materials. The depth profile in Figure 11 and the spectra subsampled from the data set used to construct the depth profile suggest an estimate for these two bulk materials is within the data set.

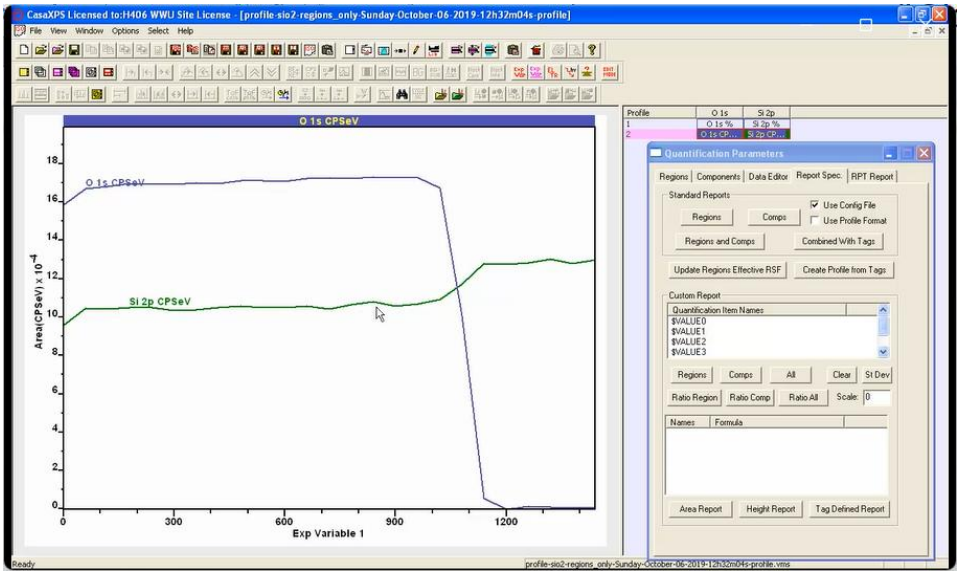

Figure 11. The second row of VAMAS blocks shown selected in the righthand-pane contain the intensity for O 1s and Si 2p photoemission. The point relevant to calculating the film thickness for SiO_2 is the change in intensity of the Si 2p CPS eV at the point in the profile where the O 1s trace goes to zero.

The plot in Figure 11 for the Si 2p CPS eV demonstrates that the rate at which Si 2p photoelectrons are emitted differs between the SiO2 compared to Si. This observation is not unexpected since one might anticipate that the number of silicon atoms per unit volume is lower in the case of SiO_2 than for pure silicon. The plot in Figure 11 also shows that the interfacial region for which Si 2p spectra include a film of oxide covering the elemental substrate is narrow. Therefore, spectra available with both oxide and elemental signal is limited in number. Moreover, when sputtering with an ion beam there is an element of doubt that the film of SiO_2 is uniform throughout this interfacial zone. The Hill Equation is most accurate if the sample can be idealised as a uniformly thick overlayer on a substrate. Furthermore, the Hill equation involves taking the ratio of the intensity of photoelectron emission from the overlayer to the corresponding intensity from the substrate. The Si 2p spectrum used in the video has the unfortunate proportions of these two intensities that are not ideal for use in the Hill equation. Preferably, the denominator in the Hill equation obtained from the substrate would be of greater magnitude. These and other reasons are the cause for uncertainty in the depth estimate shown in this video. Nevertheless, in an ideal world, the steps would provide a good estimate for the sputter rate and, if not an ideal world, certainly are useful as a vehicle for conveying data treatment in CasaXPS.

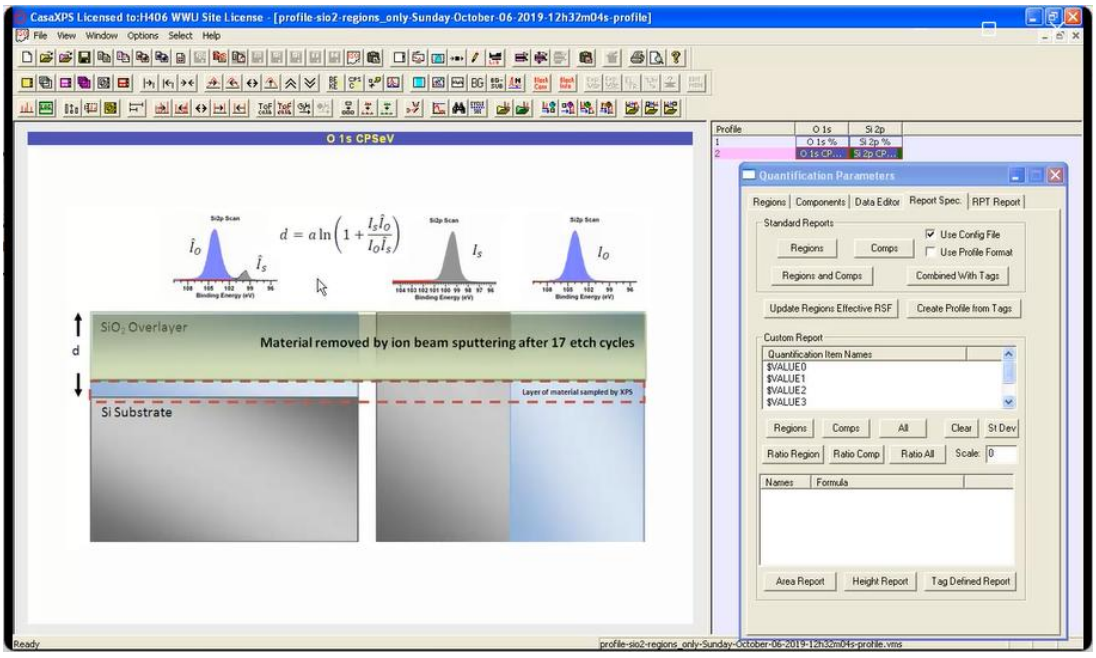

Figure 12. Illustration of the different quantities used in the Hill equation to estimate the thickness of a uniform film of SiO_2 on a substrate of Si. Spectra measured from bulk oxide and bulk elemental silicon are used to normalise the intensities measured from the sample consisting of an oxide film on elemental silicon.

The depth profile VAMAS file contains a list of Si 2p spectra as shown in Figure 13. The selected VAMAS blocks are overlaid in the active display tile in Figure 13 to illustrate the three spectra that would be required to make use of the Hill equation. The VAMAS block with experimental variable 120 seconds is chosen to represent Si 2p intensity from bulk SiO_2,

while the VAMAS block with experimental variable 1380 seconds is chosen to represent Si 2p intensity from bulk Si. The spectrum for which both SiO_2 and Si signal is evident is selected also and it is this spectrum for which a peak model is used to compute the two intensities for SiO_2 and Si shown in Figure 12 that facilitate the use of the Hill equation to measure the thickness of the SiO_2 layer at the point in the experiment after 1020 seconds of sputtering the sample with an ion gun.

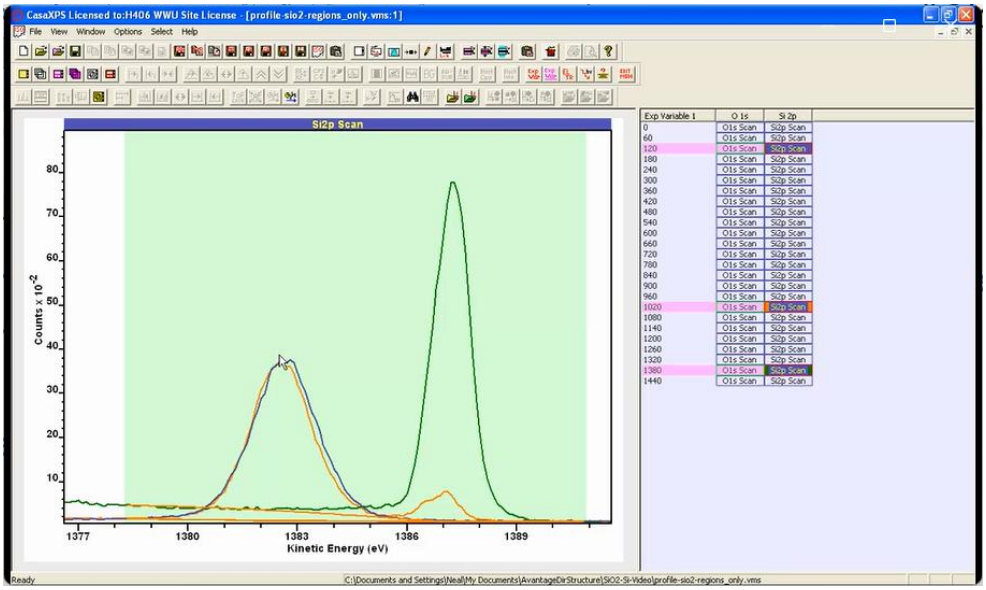

Figure 13. Three spectra displayed in the active tile are used to estimate the intensity of Si 2p measured from bulk SiO_2 and Si, and the thickness of a thin film of SiO_2 on Si.

Rather than computing the estimate for the film thickness from spectra in the original VAMAS file containing the depth profile, the three VAMAS blocks selected in Figure 13 are copied to a new VAMAS file. Once in the new VAMAS file, the VAMAS blocks can be rearranged without altering the logical structure of the depth profile that relates pairs of O 1s and Si 2p spectra with etch-times. When generating a quantification report using the Quantification Parameters dialog window, Report Spec property page, the VAMAS blocks necessary for the computation of a quantity must be aligned in a row of VAMAS blocks as seen in the righthand-pane. To align VAMAS blocks into a row of VAMAS blocks, it is necessary to assign unique element/transition fields to each VAMAS block to be placed in a row of VAMAS blocks when displayed in the righthand-pane. Further, the VAMAS blocks must also be assigned the same experimental variable value or the same label (often the sample identifier string) that is displayed when the Edit Mode toolbar button is pressed. In Figure 14, the Edit Mode is active and therefore the string “Depth Profile” assigned to each VAMAS block is used to align the VAMAS blocks into a row. However, before the VAMAS block form a row in the righthand-pane, the element/transition fields must be edited as shown in Figure 14. In the event that Edit Mode does not show the same string for VAMAS blocks as seen in the righthand-pane in Figure 14, an assignment for the sample identifier string can be made using the toolbar button indicated in Figure 14. The target arrangement

for the VAMAS blocks required by the Report Spec, Custom Report option that permits the calculation of a film thickness is illustrated in the righthand-pane of Figure 15.

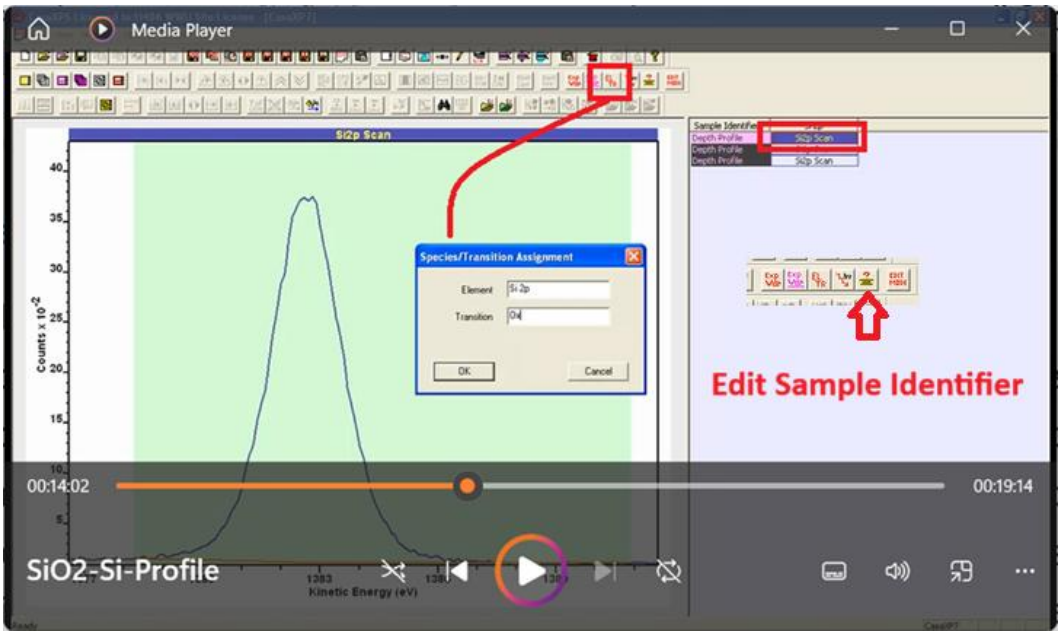

Figure 14. The element/transition string, used to separate VAMAS blocks into different columns of VAMAS blocks in the righthand-pane, is edited using the El Tr toolbar button to invoke the Species/Transition Assignment dialog window. The strings entered on the dialog window are assigned to all VAMAS blocks selected in the righthand-pane.

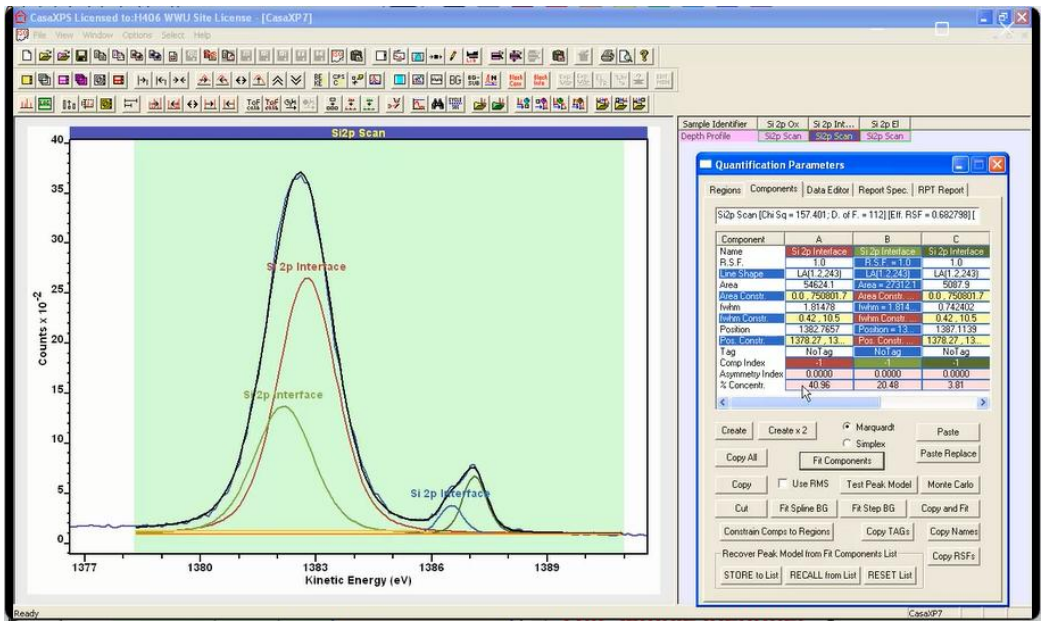

Figure 15. Peak model with constraints between optimisation parameters designed to force a fit to data that is physically meaningful.

After the VAMAS blocks are aligned ready for use by the Quantification Parameters dialog window, Report Spec property page as shown in Figure 15, the video proceeds to create a peak model for the Si 2p spectrum from the interfacial zone between the two silicon

chemistries. An important feature of a peak model is the use of constraints applied between optimisation parameters. In the absence of optimisation constraints, the mathematics of optimisation will fit spectral shapes, but more often than not, the component peaks selected by an unconstrained peak model will not reflect the true chemistry of a sample. Constraints are an essential part of building a peak model that reflects the chemical states of silicon, but more importantly, well-chosen constraints provide the rigidity in the peak model to permit meaningful measurement of relative intensity for photoelectron emission from oxide and elemental silicon. Figure 15 shows the Quantification Parameters dialog window, Components property page populated with synthetic components (bell-shaped curves and sigmoid-shaped curves) that represent photoelectron signal and the response in inelastic scattered background intensity due to emission from elemental Si 2p photoelectrons. The colours used to display in the lefthand-pane the components that define the peak model, are also used to colour the relational constraints defined between optimisation parameters. For example, Si 2p is a doublet peak. Therefore, we know from physics that Si 2p photoelectrons appear with two distinct binding energies in the proportion 1:2. Therefore, the area parameters for the component in the component list with heading labelled B is chosen to represent the less intense of the two Si 2p doublet peaks, while the component in column A represents the more intense Si 2p peak. Consequentially, the area constraint in column B is assigned the relational constraint A*0.5, thus forcing optimisation to fit the peak model to Si 2p spectra while respecting the 1:2 relationship between the Si 2p doublet peaks imposed by physics (Figure 16). Since the area constraint for the component in column B is fixed with respect to the parameter for the area in column A, the colour used for the background to the text of the area constraint in column B is the colour used to plot the component in column A in the active tile of the lefthand-pane.

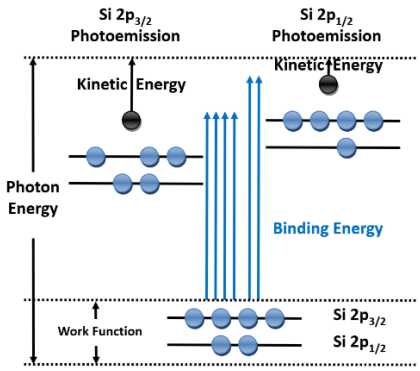

Figure 16. Quantized energy level of core-level Si 2p electrons of the neutral atom and the two possible core-level electron configurations for the ion in a state with a hole in Si 2p electrons. The hole in the ion allows coupling between the orbital angular momentum of electrons and the, so called, spin angular momentum of electrons. The consequence of the hole is the final state offers two electron configurations offset in energy, where the availability of outcomes when photoionization occurs favours the Si $2p_{3/2}$ final state by a factor of two compared to the Si $2p_{1/2}$ final state.

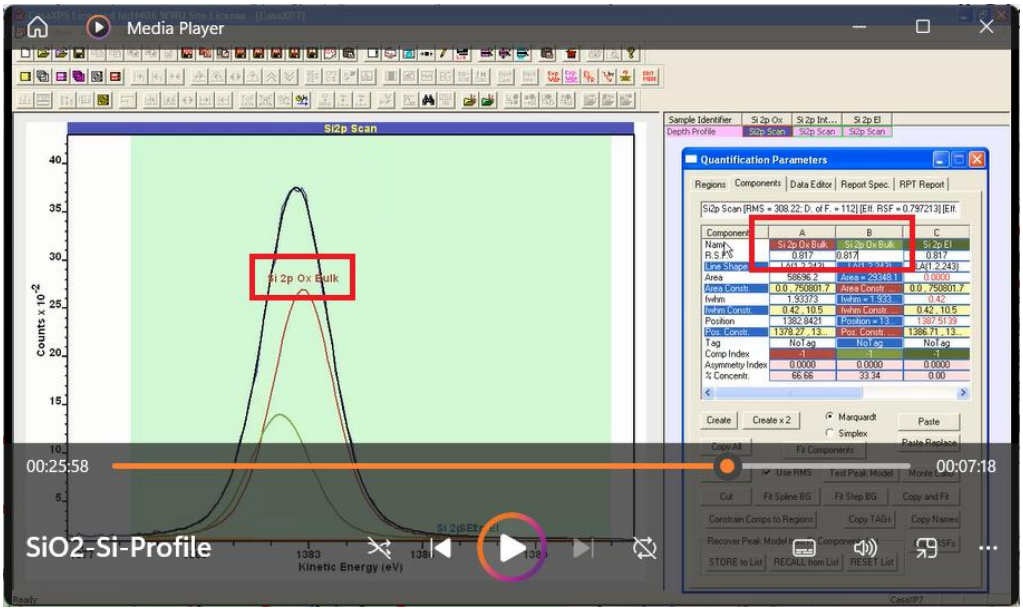

Figure 17. The Name fields for both quantification regions and components to a peak model are important when using the Custom Report. For this reason, the Name field for the regions is redefined in the video to be “Si 2p R”, while the Name fields for the different components from the oxide originating from the bulk oxide are assigned the same string “Si 2p Ox Bulk”.

The Name fields for both quantification regions and components to a peak model shown in Figure 17 are important when using the Custom Report. The variables used to construct formulae for the Custom Report are defined by these Name fields. The Name field also alters the way intensities are gathered from regions and components. Name fields that are identical are summed by the Custom Report. For this reason, the Name fields must be unique unless it is the intention to add together intensities derived from different regions and or components. Hence, the Name field for the region is redefined in the video to be “Si 2p R”, while the Name fields for the different components from the oxide originating from the bulk oxide are assigned the same string “Si 2p Ox Bulk”.

The expression in Figure 18, that derives from the Hill equation, includes the effective attenuation length for electrons with kinetic energy corresponding to Si 2p scattered by photons of energy 1486.7 eV within SiO_2, and the logarithmic expression therein uses intensities extracted from the peak models defined on each of the three spectra selected in Figure 18. The take-off-angle for electrons is perpendicular to the sample surface, therefore the angular dependence within the Hill equation, for this experiment, is unity.

The dialog window shown in Figure 18 is designed to edit an entry in the Names/Formula table. However, before an entry in the Names/Formula table can be edited an entry must be placed into the table by other means. The buttons between the Quantification Item Names table and the Names/Formula table in the Custom Report will search for unique names defined for regions, components or regions and components defined on the VAMAS blocks currently selected in the righthand-pane and for each unique name found an entry will be

created in the Names/Formula table. Alternatively, to add an entry to the Names/Formula table the button header to the Names column of the Names/Formula table can be pressed. Figure 19 illustrates the button header used to create a new entry in the Names/Formula table. The dialog window shown in Figure 18 is invoked by placing the cursor over a string in the column labelled Names before using the righthand mouse button. The Ok button on the dialog window in Figure 18 updates the entry used to invoke the dialog window (Figure 20). The entry can be deleted by exiting the dialog window via the Delete button, or an additional entry is created using the edited Name and Formula on the dialog window by exiting the dialog window using the Insert button as seen in Figure 18.

An important point to emphasise is that regardless of whether the Name field originates from a region or a component, any region or component with the same name defined on the selected VAMAS blocks, results in the summation of intensity gathered from regions and components for use in the formulae in the Names/Formula table. Therefore, it is important to name regions differently from components, unless it is intended to sum intensities using both regions and components.

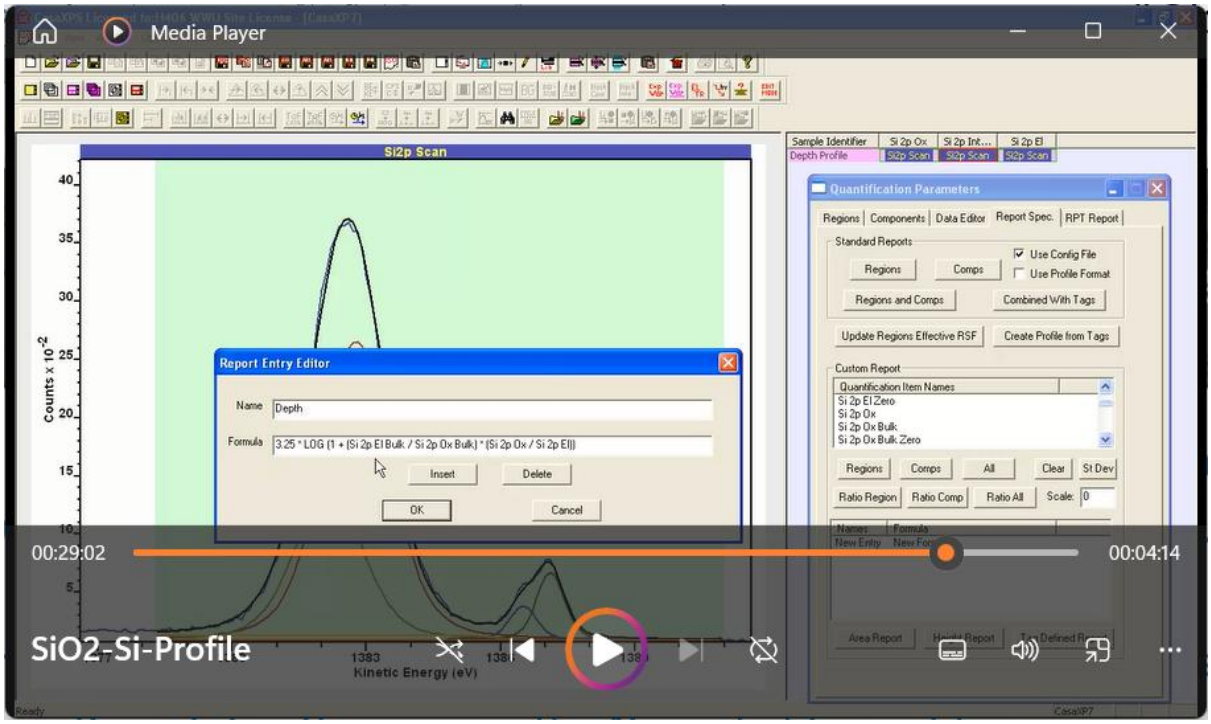

Figure 18. The Custom Report section of the Quantification Parameters dialog window, Report Spec property page makes use of the names assigned to the Si 2p components to create an expression for the Hill equation, specific to SiO_2. The effective attenuation length (nm) is obtained for SiO_2 using the formula published by Martin Seah. For different materials and photoelectrons with different kinetic energy, the effective attenuation length is different from the value used herein.

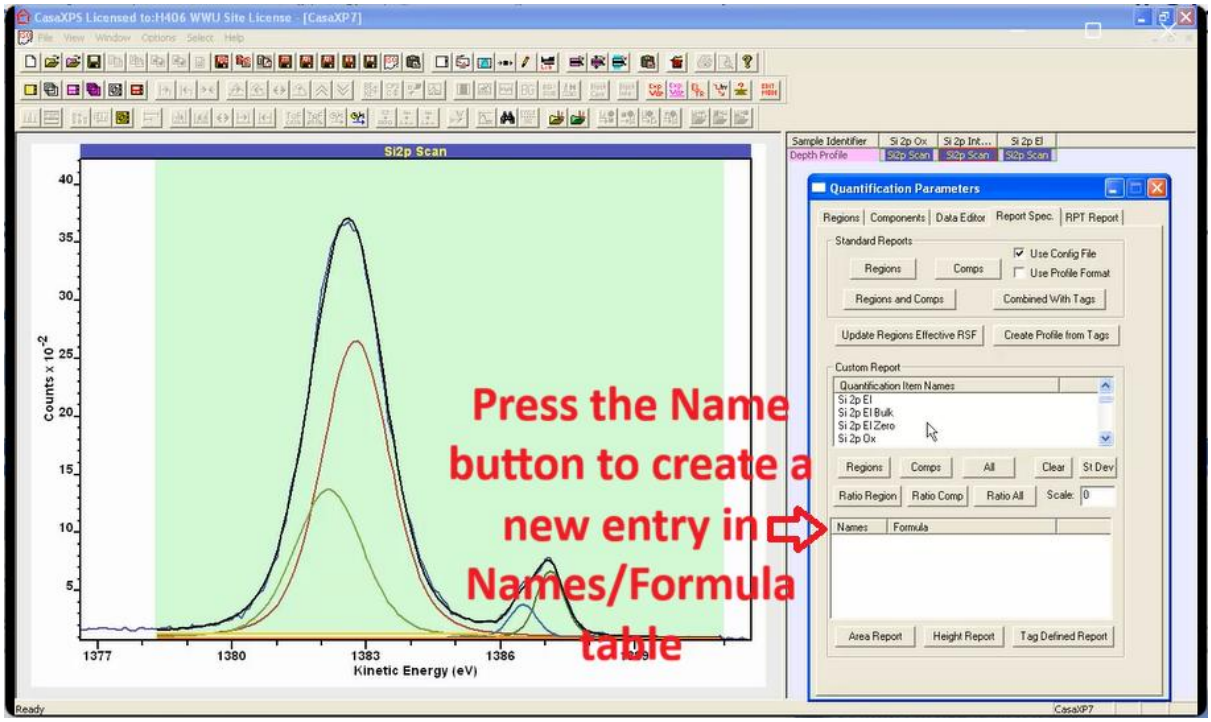

Figure 19. Initially the Names/Formula table is empty. To create an entry in the table, press the indicated column header button labelled *Names*. Once an entry is created, the name and formula can be edited to specify the Hill equation in terms of the names for components to peak models defined on the selected VAMAS blocks. The dialog window used to edit the name and formula for the newly created table entry (shown in Figure 18) is invoked by placing the cursor over the newly created name (*New Entry*) and a right-click of the mouse button.

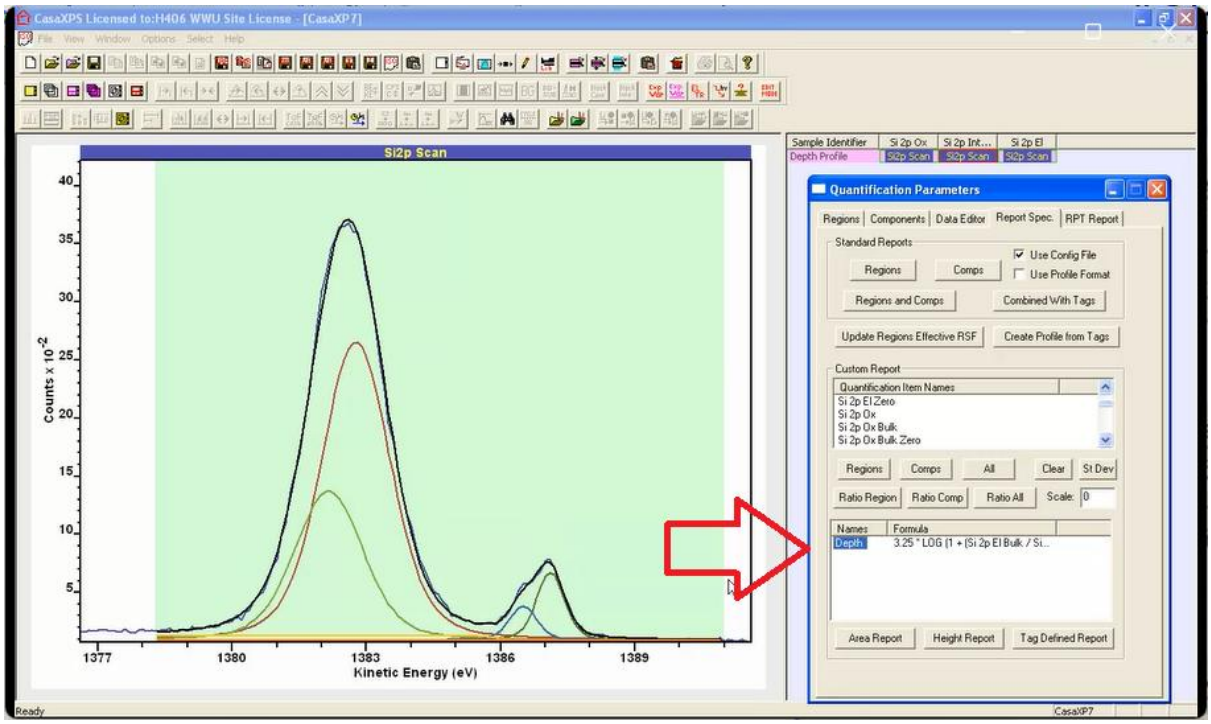

Figure 20. On pressing the Ok button on the dialog window, the Names/Formula table is updated from the Report Entry Editor dialog window shown in Figure 18.

Once the Names/Formula table is prepared as shown in Figure 20 with the name of Depth Profile and the formula constructed from the component Name field defined on the selected VAMAS blocks, pressing the Area Report button of the Custom Report (Figure 21) creates a text report window, where the depth is calculated from the formula as indicated. When using a complex formula, such as the Hill equation, the units presented in the header, namely CPS eV in Figure 21, indicate the units of the variables used in the expression, not the units for the outcome of the formula, which in the case of the Hill equation is the units of the effective attenuation length i.e. nanometres.

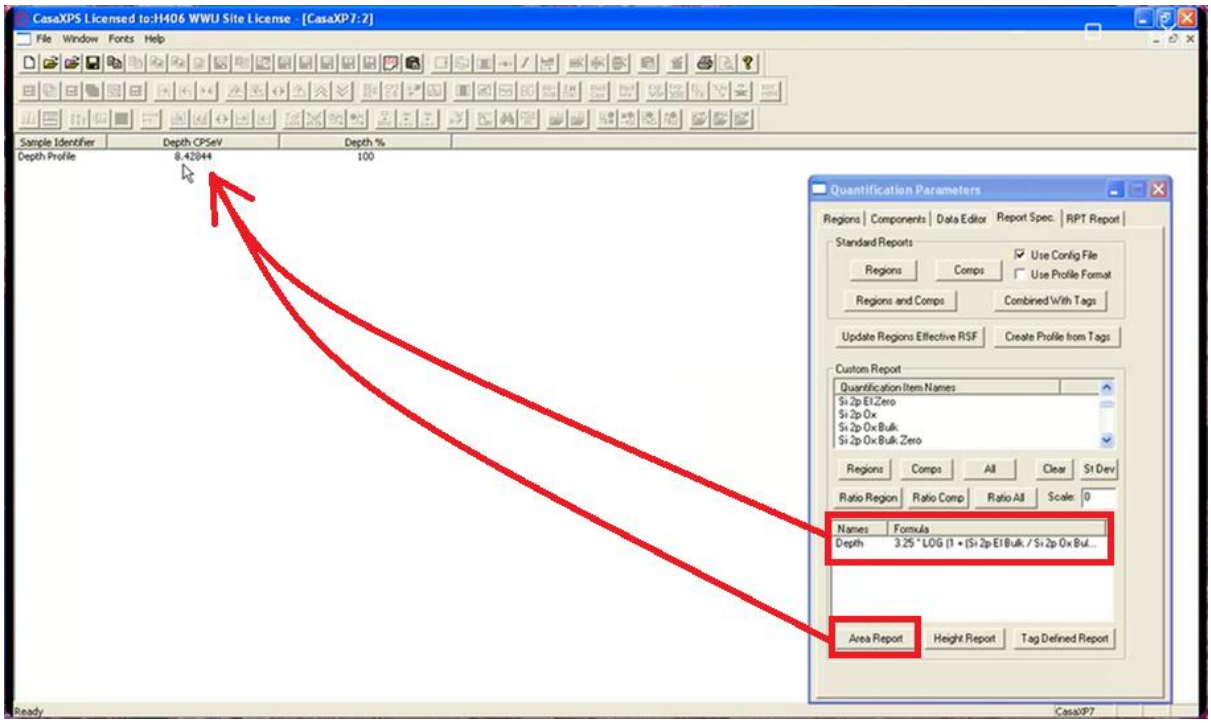

Figure 21. Given the formula for the Hill equation and the selection of VAMAS blocks in Figure 20, the outcome of pressing the Area Report button is a table containing the depth in nanometres computed from the Hill equation for the SiO_2 film at the point in the depth profile from which the interface spectrum was selected.

The experimental variable for the VAMAS blocks from which a depth profile is created was initially etch-time in seconds. However, the objective for the experiment is to estimate the thickness of the SiO_2 film on Si. Therefore, the experimental variable needs to be converted from etch-time to depth in nanometres, which can be achieved by calculating the rate at which the ion gun removes SiO_2 by sputtering material from the surface. So, given the point at which elemental silicon is observable in Si 2p spectra for the first time, and the point at which elemental silicon is the dominant signal in Si 2p spectra, the time interval estimated for these two states of the sample provides an estimate for the time taken to remove a film of SiO_2 of known thickness. Figure 22 illustrates a visual means for estimating the time to

remove a film of SiO_2 with thickness 8.4 nm. The estimated sputter rate is 0.07 nms^{-1} (Figure 22).

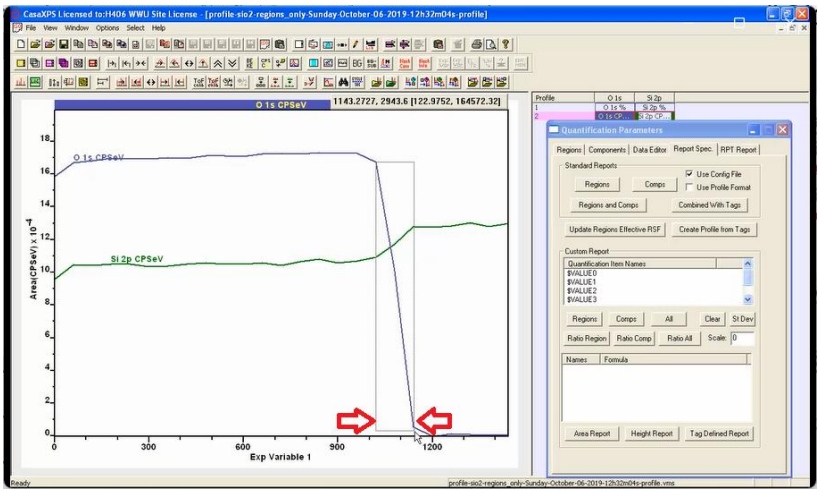

Figure 22. Using the previously prepared depth profile, an estimate is determined for the time taken to sputter the surface initially of thickness calculated in Figure 21, namely 8.4 nm until the Si substrate is mostly exposed. The estimated time to remove 8.4 nm of SiO_2 is 120 seconds, therefore a sputter rate for SiO_2 is approximated using 0.07 nms^{-1}.

Given the sputter rate for SiO_2, which may be obtained by sputtering a standard SiO_2 material and measuring the crater depth or, in this case, using XPS to estimate the sputter rate, the experimental variable for the spectra is converted from etch-time to nanometres using the dialog window illustrated in Figure 23.

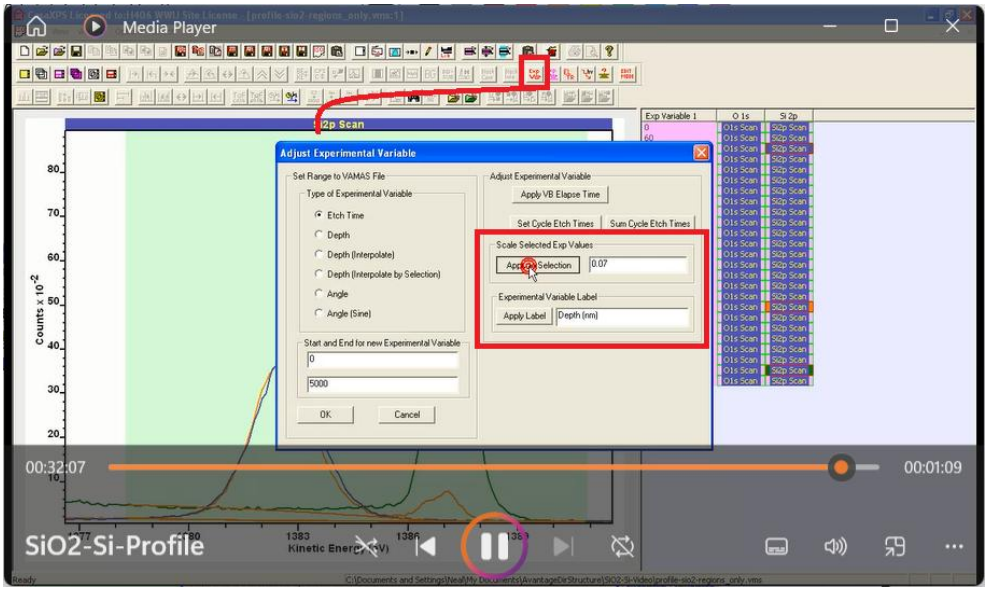

Figure 23. Converting the experimental variable from etch-time to depth in nanometres is performed using the dialog window invoked by the indicated toolbar button. The *Scale Selected Exp Values* section allows the sputter rate and a new label for the experimental variable to be assigned for each VAMAS block selected in the righthand-pane.

Reconstruction of a depth profile VAMAS file (Figure 24) from the VAMAS blocks now adjusted from etch time in seconds to depth in nanometres is achieved using the exact same steps illustrated in Figure 9.

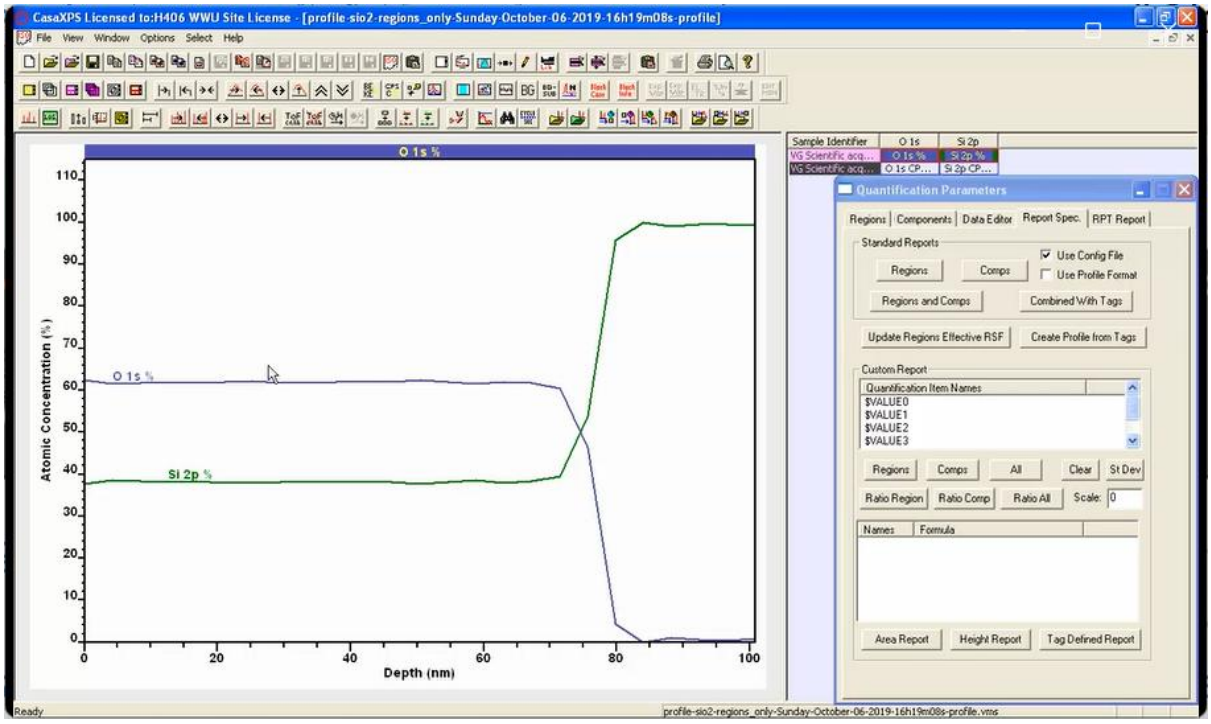

Figure 24. Depth profile created from the VAMAS file shown in Figure 23 following converting the experimental variable from etch-time in seconds to nanometres.