Dynamic SIMS

Calibration of SIMS depth profiles

SIMS depth profiles are calibrated from counts per cycle/cycles to atomic density/depth using Relative Sensitivity Factors (RSF) and sputter rates. Computation of these conversion factors and subsequent assignment to complex matrix structures is performed on the Dynamic SIMS dialog window available from the SIMS toolbar Image. The SIMS toolbar may be displayed using the View menu on the CasaXPS Main Window.

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Figure	1	SIMS	toolbar
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Logical Structure of a SIMS Depth Profile within CasaXPS

A depth profile is a collection of VAMAS block all assigned to the same experimental variable value; typically the experimental variable will be an index number for a given file of data. There may be more than one profile per VAMAS file, where each profile will occupy a row as viewed via the right hand side VAMAS file browser pane. For each VAMAS block within a raw depth profile, a number of corresponding variables are setup to offer fields for use in the quantification step. The important fields for quantification are displayed in the Matrix Index table on the Dynamic SIMS dialog window (Figure 2).

Dynamic SIMS						
Calibration						
Define Interface	D	efine Matrix	M [3]	[3]		
Define Surf/BG	Matrix In.	Interface	RSF	Sputter	C 🔨	
Dose (atoms/cm2):	Ga [2] Ga [2]	69G [0] 69G [0]	1.4e+019 1.4e+019	3.3333e 3.3333e	1: 1.	
1.0000e+000	Ga [2] Ga [2]	69G [0] 69G [0]	1.4e+019 1.4e+019	3.3333e 3.3333e	1:	
Depth (nm):	Ga [2] Ga [2]	A [1] A [1]	1e+019 1e+019	2.5e-008 2.5e-008	3	
1.0000e+007	Ga [2] Ga [2]	A [1] A [1]	1e+019 1e+019	2.5e-008 2.5e-008	4	
Subtract BG	Ga [2]	A [1]	1e+019	2.5e-008	4	
Elemental RSF	Bulk Dope	ed (atoms/cm3	3): 1.0000e	+000	_	
Compute RSF	Use f	Bulk Doped	Compute S	Sputter Rate		
RSF: 1.0000e+	-019	Sputter Rat	e(cm/s): 2.	5000e-008		
Apply RSF/SR to M	latrix App	by RSF/SR to	Interface	Restore RSI	F/SR	
Depth Profile Calibra	tion					
Calibrate Dept	n Profile	Normalise to Matrix		Interface Statistics		
Calibrate All P	V Use Nar	o metres	Profile Statistics			

Figure 2: Dynamic SIMS Calibration Dialog Window.

Computation of RSF and Sputter Rate Values

RSF values are computed from standard materials using one of three approaches:

- 1. Matrix, dopant and crater depth.
- 2. Matrix, known bulk doped atomic density and crater depth
- 3. Interface assignment with respect to depth and atomic density.

The computation of the RSF requires the determination of values from the Matrix signal and also the Implant. To support the determination of these quantities the matrices within a profile must be identified and a pair of regions defined to specify the surface zone as well as the appropriate background signal for a given mass.

Defining the matrix is achieved as follows:

Single matrix materials

- 1. Display the matrix signal for each profile in the active display tile.
- 2. Press the Define Matrix button on the Calibration property page on the Dynamic SIMS dialog window. A pop-up window will inform you that no matrix index is selected and asked whether the displayed matrix should be applied to all Cycles. Answer by pressing the Yes button. To avoid the warning message, before pressing the Define Matrix push button, first select all the table entries by pressing the header button for the column labelled Matrix Index. If there are any rows currently selected it will be necessary to de-select these rows before pressing the header Matrix Index.

If the file contains more than one depth profile and the matrix for each profile is overlaid in the active tile, then the operation of defining the matrix for each depth profile is performed in one go.



Figure 3

Layered materials

Complex structure in a material requires the definition of both the matrix material and also the layer structure. The procedure for defining the matrix and also the a layer is identical except for different buttons are used to make the assignment.

- 1. Display the signal for one mass in the active display tile.
- 2. Either using the table or the mouse (see below), select ranges of cycles within the Matrix Index column of the table on the Dynamic SIMS dialog window.
- 3. Press the Define Matrix or Define Interface button (Figure 2 and Figure 3) depending on whether the matrix or a layer is being assigned. Only those cycles selected in the table will be assigned to each element within the experiment.

The matrix/layer structure is used to update the appropriate cycles with the RSF and sputter rates.

Selecting rows within the Matrix Index table is achieved using the table together with the Shift and Control Keys. Alternatively, the selection can be defined using the active tile and the mouse. When the Shift Key is held down and the left mouse button is used to drag over the display, the set of cycles corresponding to those lying between the vertical cursors (Figure 3) will be selected in the Matrix Index table. This aids the identification of layered structures viewed via the matrix signal trace. Once a set of layers are so indicated, the assignment is made by pressing the Define Matrix or Define Interface button.

Defining the Surface and Background Regions:

- 1. Display any number of VAMAS blocks in the active display tile.
- 2. Press the Define Surf/BG button (Figure 2).

Two regions will appear on each profile; the left most region indicates the peak and should be adjusted to start just after cycles associated with any surface spike. The second right-most region defines the background to the tail of an implant. Both regions can be adjusted using the Quantification Parameters dialog window when viewing the Regions property page (available from the Option menu). The left mouse button may be used to drag the start and end position of these regions whenever the Region property page is active. Adjustment under mouse control is available when grey vertical lines at either end of the regions are displayed which appear when the Region property page is active.

Once the matrix and regions have been defined, the RSF can be computed by the appropriate method:

- Either: enter the Implant dose in Atoms/cm² and the measured crater depth in nanometres then press the Compute RSF button and also the Compute Sputter Rate buttons. Pressing these buttons will result in the corresponding values appearing in the boxes below the buttons.
- Alternatively, if a bulk doped standard is in use, tick the box labelled **Use Bulk Doped** and enter the known atom density into the above data input field. Both the implant and matrix require regions when a bulk doped standard is used to compute the RSF.
- The third method for computing the RSF is via a known implant depth and atom density. The button to the right of the Depth field, namely, Depth (m): _____ results in a dialog window in which a depth and/or a peak intensity can be entered (Figure 4). The position of the implant is defined using the Matrix Index table by making a single selection in that table. The appropriate cycle can be identified by left-clicking on the peak in the left-hand-side active tile. The Matrix Index table scrolls to show the cycle corresponding to the mouse selection and the table entry is therefore offered for selection prior to invoking the Define Depth by Cycle dialog window in Figure 4. If the correct depth and corresponding atoms per cc are entered, the Calc RSF tick box is ticked and the OK button is pressed, the RSF, Depth and Sputter Rate fields will be updated.

Define Depth b	y Cycle	X
Cycle:	299	OK)
Depth (nm):	1000000	Cancel
Atom/cm3:	1	Calc RSF
4		

Figure 4

Once an RSF is computed and the appropriate Sputter Rate entered for an implant in a given matrix, the profile can be update with these values: select a cycle from the Matrix Index table with the appropriate the matrix entry and press either the Apply RSF/SR to Matrix button or the Apply RSF/SR to Interface button. Each cycle within the profile with the same entry as the selected matrix index will be updated with both the Sputter Rate and the RSF. If the material is a multilayer structure the procedure should be repeated for each layer, where the RSF and Sputter Rates are first determined from a standard profile. An RSF/Sputter Rate pair can be extracted from another profile by first displaying the profile, making a selection in the Matrix Index table and pressing the RSF/SR button. The RSF/Sputter Rate from the indicated matrix index will be entered into the fields on the dialog window, thus allowing the unknown to be subsequently displayed and these restored values from the standard used to update the unknown profile. Note, the Dose and depth for single matrix material are computed when the **Apply to Selected Matrix** button is pressed.

Once RSF and Sputter Rates have been assigned to each depth profile, the data are calibrated by pressing the Calibrate Depth Profile button. If multiple profiles are prepared and overlaid in the active tile, pressing the Calibrate All Profiles button results in each profile, so selected, being calibrated and entered into a single Experiment Frame. The depth scale units must be selected prior to calibration using the tick box **Use** Nanometres.

Note: If normalization to the matrix is not requires, it is necessary to compute the RSF with the same selection of the Normalize tick box.

Depth Profile Statistics: Areal Density and Decay Length

Areal Density and Decay Length are computed as part of the Depth Profile Statistics. The procedure for calculating these statistics requires a pair of cursors to be defined on the displayed profile in the active tile. The aim is to mark the region over which the profile peak appears. To mark the cursors on the profile: hold the Shift Key down and drag a box starting from the left of the peak and ending at the right-hand end with the mouse positioned at the intensity of the background. On pressing the Profile Statistics button (Figure 2) a dialog window appears showing the current text in the VAMAS block comment plus a set of lines offering the new calculated profile statistics. If it is desired to include these new lines in the VAMAS block comment, then the OK button should be pressed, otherwise the Cancel button will exit without altering the VAMAS block comment. Note, the text in the VAMAS block comment can be edited within this window leaving only the information so required.

Maintaining Standards Library Files

Once standards have been prepared and RSF/Sputter Rates computed, these depth profiles can be moved to other files containing profiles from standards. The toolbar buttons is allow VAMAS blocks to be copied

into an existing file and also delete from a file. Once a number of standard material profiles are located in a single file, the *button offers a means of searching the strings within a VAMAS block comment and those matched are both selected in the right-hand side of the Experiment Frame and are also displayed in the scrolled list of display tiles. VAMAS block comments can be edited using the <i>button button.*

A Multi-Layer Example

In this example, the desired result is a plot of atomic density verses depth for Mg. To achieve this end and owing to the layered structure, four masses were monitored, where two labeled 69G and A define the layer structure while the trace labeled Ga represents a constant matrix signal, to which the Mg signal is normalized.



Figure 5

Step 1: Define the Matrix

Display the matrix, namely, Ga in the Active Tile. The block id plus the VAMAS Block index for the trace will appear on the Dynamic SIMS dialog window (indicated within the red box). Select all the cycles under the Matrix Index column in the table on the Dynamic SIMS dialog window and press the Define Matrix button (also indicated within the red box). The selected entries under the Matrix Index column will change to say Ga [2] and thereby showing the matrix is defined.







Step 2: Define the Layer Structure

The material is GaN : AlGaN : GaN in structure (Dr Shadi Shahedipour, University of Albany, New York) therefore step 2 requires the definition of the interfaces. The AlGaN layer is characterized by the trace labeled A in Figure 3. To define a layer within a profile, the signal shown in Figure 3 is used to select the set of cycles recorded between the two interfaces. Before using the mouse to indicate the interfaces, ensure there are no selected cycles in the table on the Dynamic SIMS dialog window. Clicking on any column away from the Matrix Index column will de-select all cycles. Repeated use of the mouse will add to the current selection, allowing complex multilayer materials to be specified.

Mark the AlGaN layer by holding the Shift-Key down and then dragging a box from the left to the right of the AlGaN peak. The result of such an action is shown in Figure 3. All the cycles within the table on the Dynamic SIMS dialog window between the vertical cursors shown on Figure 3 are selected by the mouse action and so pressing the **Define Interface** button on the same property page will cause the Interface column in the table to be updated.

Step 3: Enter RSF and Sputter Rate Values

In this example the RSF and Sputter Rate for the two layers are assumed to be known. All that is required is to add sputter rates and RSF for each of the three layers; the values are entered on the Dynamic SIMS property page in Figure 2, a given matrix or interface cycle is selected and the table entries corresponding matrix or interface updated by pressing **Apply RSF/SR to Matrix** or **Apply RSF/SR to Interface**, as desired. In this example, two RSF and SR pairs are entered corresponding to the GaN and AlGaN layers. Since the matrix does not define the layer structure, the assignments are made by using the **Apply RSF/SR to Interface** button. After displaying the Mg trace in the Active Tile the RSF/SR can be entered. Firstly, both the GaN layers are assigned by selecting one cycle for which the interface button. Each cycle previously designated as part of the 69G [0] layer will receive the RSF/SR pair. Similarly, the AlGaN RSF/SR to Interface button pressed a second time. Again, each cycle designated as Interface A [1] will receive the RSF/SR pair. (Figure 7)

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Figure 7

Step 4: Calibrate Mg Profile

Calibration is performed by displaying the profile in the Active Tile and pressing the Calibrate Depth Profile button in Figure 2.

In this example, the only mass for which RSF/SR pairs are entered is Mg. The SR are automatically assigned to all masses, however the RSF values for masses other than Mg remain set equal to unity. A consequence of leaving an RSF equal to unity is that on Calibration to atomic density and depth, masses for which the RSF is equal to unity will be scaled to the atomic density range of any properly calibrated masses. This allows an overlay with respect to the calibrated traces, without requiring the RSF for all masses to be assigned prior to calibration. Counts per second traces are available in the calibrated Experiment Frame as the second corresponding variable (Ctrl PageUp/Crtl Page Down).





Figure 8: Calibrated Mg profile with scaled A/Ga/69G data.

An Example of Computing an RSF

The profile in Figure 9 was obtained from GaN undoped epi growth ion implanted with ²⁴Mg at a dose of 1.0e15 atoms per cm². The depth at the peak of the Mg counts is 77 nm. Computation of an appropriate RSF is performed as follows:

Step 1: Define the Matrix

Display the Ga2 matrix profile in the Active Tile, press the header button labeled Matrix Index in the table to select all cycles and press the Define Matrix push button on the Dynamic SIMS dialog window. The table on the same dialog window will update to show that the Matrix index for each cycle is now assigned to the Ga2 profile.





Step 2: Define the Surface Layers and also the Background for the Mg Profile

Display the Mg profile in the Active Tile and press the button labeled Define Surf/BG. Two regions are created on the Mg profile. The left-most end of the left-most region defines the surface layers, while the background to the right-most of the two regions estimates the background to the Mg signal.

Step 3: Define the Depth Scale

In this example, the depth scale is defined to be 77nm at the maximum signal for the Mg profile. Using the left-mouse button, click on the profile to indicate the position of the Mg maximum values. The table entries on the Dynamic SIMS dialog window will scroll so that the cycle, corresponding to the position of the vertical cursor, is located at the top of the visible portion of the list. Select the entry at the top of the visible portion and press the button next to the Dept (nm): label (Figure 10). A dialog window appears in which the selected cycle index in already entered and a text-field for the Depth (nm) corresponding to the indicated cycle can be input. On pressing the OK button, the Dynamic SIMS dialog window in updated with the Depth computed from the **Define Depth by Cycle** dialog window values.



Figure 10

Step 4: Enter the Dose and Compute the RSF

Enter the dose in atoms per cm^2 on the Dynamic SIMS dialog window and press the button labeled **Compute RSF**. If the elemental RSF is required, the tick-box just above the Compute RSF button should be ticked (Figure 10).

Step 5: Calibrate the Mg Profile

Once the RSF is computed and the sputter rate updated, the values for each cycle corresponding to the Mg profile (currently displayed in the Active Tile) must be updated. In this example, the assignment for the matrix is sufficient to target the cycles for which RSF and sputter rates must be applied. Simply select any cycle using the Matrix Index column in the table and press the **Apply RSF/SR to Matrix** button. Since all the cycles are defined to have the same matrix, the table for the Mg profile will contain values for the RSF and sputter rate throughout. To calibrate the profile, press the button labeled **Calibrate Profile**.

The calibrated profile for Mg is shown in Figure 11. Note that the Profile Statistics button (Figure 2) has been used to create a VAMAS block comment showing the Areal Density and Decay Length for the Mg profile. Also note how the profiles for which no RSF is specified are scaled to allow their visualization within the same scale as the calibrated Mg profile.



Mg Areal Density 1.031e+015 atoms/cm2, Background Intensity = 3.844e+017 atoms/cm3 Peak Height 1.082e+020 atoms/cm3, Peak depth 78.228 nm Decay Length (1/e):46.633 nm (1/10):107.38 nm



Figure 11