IR-VASE® Reflectance measurements with baseline reference-sample correction

Contents

Baseline reference sample correction for the IR-VASE®

Why Reference-sample baseline correction?

For *reflectance* measurements, the "straight through" baseline measurement method generally does not produce accurate data. That is because it does not account for shifts in beam trajectory that occur as the instrument goniometers rotate from the straight-through orientation to some other angle. Furthermore, the beam profile, which is non-symmetric, is reversed upon reflection. Both the shift in trajectory and image reversal can cause a small portion of the beam to miss the detector aperture[1]. This can cause systematic errors of 1% or more.

A. Intensities: sample, baseline & recorded

For reflectance and transmittance measurements, WVASE® and WVASE-IR® always records the intensity value ($I_{recorded}$) derived from the ratio of two measured intensities:

$$I_{recorded} = I_{sample} / I_{bl} \tag{1}$$

I_{sample} is the reflected (or transmitted) intensity measured from the sample under test, and I_{bl} is the measured baseline intensity under the same polarization conditions (p- or s-polarized incident light, p- or s-polarized detector).

Dividing I_{sample} by I_{bl} corrects for variations in source intensity and detector sensitivity vs. wavelength, provided these do not change in the time between the background and sample-under-test measurements[2].

Baseline intensities can be acquired using either the "straight-through" configuration (no sample in beam path, detector at 180° position), or from a reference sample.

B. "straight-through" baseline measurements

In the "straight-through" configuration the baseline "sample" is assumed to be the ambient, and $I_{bl} = 1$. In this circumstance, the reflectance R (or transmittance T) for the sample under test is simply the recorded intensity:

$$R(or\ T) = I_{recorded} \tag{2}$$

R (T) can be of any polarization type – *ARpp, ARss, ARps, ARsp, etc.* (*ATpp, ATss, ATsp, etc.*).

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[1] For ellipsometry, the detector aperture can be smaller than the beam diameter because it does not need to collect the entire beam to measure a change in polarization. Ideally, for R/T measurements the detector aperture should be slightly larger than the beam.

[2] Baseline measurements do not correct for non-specular scattering, or for "lensing" effects due to wedged or curved substrates.

The "straight-through" baseline measurement works fairly well for normal-incidence transmittance measurements, because it accounts for variations in source intensity and detector sensitivity[2], and $T = I_{recorded}$.

For IRVASE® measurements the user can choose between a "straight-through" configuration or a reference sample for baseline measurements.

C. Baseline correction using reference sample

In order to account for these errors caused by beam trajectory and image reversal errors, baseline data can be acquired from a reference sample of known reflectance.

When baseline data are acquired from a baseline reference sample of known reflectance, $I_{recorded} = I_{sample} / I_{bl}$ as in equation (1). The reflectance R (*ARpp*, *ARss*, *etc.*) is then calculated from

$$R(or\ T) = I_{bl-mod} \cdot I_{reported} \tag{3}$$

I_{bl-mod} is the baseline intensity calculated from an optical model of the baseline reference sample (the assumption being that the optical model correctly predicts the I_{bl-mod}). Note that in the "straight-through" configuration, the baseline sample is "void", therefore $I_{bl-mod} = 1$ and Equation (3) becomes Equation (2).

The WVASE® *rt_baseline* layer

The WVASE® *rt_baseline.mat* layer is a special "directive" layer (see box below) that modifies the generated R-T data based on calculated optical model of the baseline reference sample (I_{bl-mod}). There are two calculation modes:

- ***The 'Generate Corrected R-T Data' mode*** generates corrected R-T data from the reported intensity data, using Equation (3). That is:

  $$R(or\ T)_{gen-corr} = I_{bl-mod} \cdot I_{reported} \tag{4}$$

  The "Generate Corrected R-T Data" mode does not require any model for the test sample; it only requires an accurate baseline model. The user can then save the corrected data after it has been generated in the Generated Data window.

- ***The 'Sample Analysis' mode*** alters the generated R-T data by dividing the model R-T values by I_{bl-mod}. That is,

  $$R(or\ T)_{gen-anal} = I_{mod} / I_{bl-mod} \tag{5}$$

  If the goal is analyze the test sample using WVASE®, the "Sample Analysis" mode allows the user to bypass saving the corrected R-T data prior to analysis.

"Directive" layers

Layers such as *rt_baseline.mat* are not layers in the usual sense – they have no "thickness" or "optical constants". They are best described as directives that instruct WVASE® to operate on the model or generated data in certain ways. Directive layers like *rt_baseline* can co-exist in the same model window with any standard layers such as *si_jaw.mat*, etc.

The instructions contained in a directive layer are executed independently from whatever standard layers that are in the same model window. Conversely, WVASE® ignores the directive layers when it calculates the model's Jones matrix quantities using the thickness and optical functions of the standard layers.

In the case of *rt_baseline*, WVASE® is instructed to modify ("correct") the generated R-T data using I_{bl-mod} calculated from a Baseline model.

Corrected-reflectance data acquisition

A. Acquire ellipsometric data from reference sample

Acquire ellipsometric data from the base-line reference sample. Ellipsometric data should be acquired using the optimum incident angles and other measurement parameters – *there is no need to acquire* *ellipsometric* *data at the same angle(s) as the reflectance measurements*. The model obtained from ellipsometric (SE) analysis must be sufficiently accurate to generate the correct reference sample reflectance at any angle.

For the very best results, do not move thereference sample until the baseline data are acquired (step B).

This step can be skipped if the optical model of the baseline reference sample has already been determined.

B. Acquire baseline reflectance data from baseline-reference sample

B1. Mount and align the baseline-reference sample.

For the very best results, the reference sample should not be moved between the SE data acquisition (step A above) and this step.

B2. Make sure that the detector aperture is completely open.

B3. Measure Baseline data from the same sample, using the same wavelength range, step size and data Baseline Polarizer Setting (*0° & 90°,-45° & +45°, Single User Value.*) that will be used for the unknown sample measurement.

For the best results, the baseline data should be obtained at the same angle(s) used for the unknown sample measurements. If this is not practical, try to use an angle that is in the center of the angular range for the unknown sample measurement[3].

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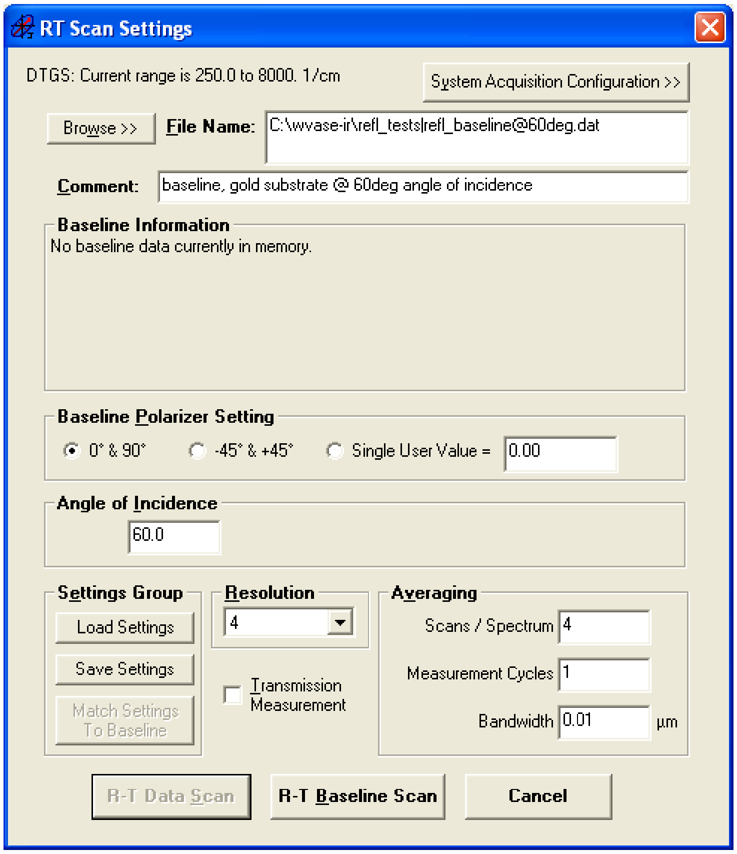
[3] The angular dependence of the reference-sample baseline correction depends on the ellipsometer's current state of alignment etc. Therefore, the user is encouraged to determine the amount of angular dependence by using the reference sample itself as the "unknown" sample – simply leave the reference sample in place and acquire reflectance data using the R-T Data Scan button. Ideally, the resulting reflectance values should all equal 1.0. Any systematic deviations from that value are an indication error, which includes systematic error due to the angle of incidence variation.



DTGS: Current range is 250.0 to 8000. 1/cm

File Name: C:\wvase-ir\refl_tests\refl_baseline@60deg.dat

Comment: baseline, gold substrate @ 60deg angle of incidence

Baseline Information

No baseline data currently in memory.

Baseline Polarizer Setting

● 0° & 90° ○ -45° & +45° ○ Single User Value = 0.00

Angle of Incidence 60.0

Resolution 4

☐ Transmission Measurement

Averaging

Scans / Spectrum 4

Measurement Cycles 1

Bandwidth 0.01 µm

Figure 1. R-T Scan Settings dialog box.

C. Measure reflectance data from test sample

The sample under test should be measured as soon as possible after the baseline measurement is made, in order to minimize the effects of time-dependent variations in source intensity, detector gain, etc.

IR-VASE® instruments will also be subject to changes in ambient gas absorption around the sample, especially CO_2 *and* H_2O*.*

C1. Mount and align the test sample. *Both the reference and baseline samples should be carefully aligned, as this directly affects the beam trajectory and therefore the accuracy of the reflectance measurement.*

C2. Ensure that detector aperture is completely open.

C3. Measure the test sample.

- Use the same wavelength range, resolution and Baseline Polarizer Setting (*0° & 90°,-45° & +45°, Single User Value.*) that was used for the baseline measurement.
- Enter a file name that is different from the baseline file name.
- When ready, select the “R-T Data Scan’ button (lower left corner of R-T Scan Setting dialog box, Figure 1).

Analyzing results with the *rt_baseline* layer

After data acquisition, the steps are as follows:

Develop a reference sample model. The *rt_baseline* layer uses this model to generate the expected baseline reflectance ($I_{bl\text{-}mod}$ in equation (3)) for the desired angles of incidence.

Once this model is finished, the user can follow either of two procedures:

1.1A: Generate corrected R-T data. The generate corrected R-T mode uses equation (3) above to calculate the correct *R(or T)* data, and save it.

B: Analyze R-T data for the test sample. The "Sample Analysis" mode allows the user to directly analyze the uncorrected R-T data from the sample under test, without having to generate and save the corrected R-T data.

Analyze SE data to determine baseline reference sample model

This model is used by the rt_baseline *layer to generate the baseline reflectance at various angles.*

First, analyze the ellipsometric data acquired from the baseline reference sample in the usual way to obtain its correct optical model.

Next, save the model[4] when finished. It will be used for generating corrected data or analyzing data from the test sample. Alternately, save the entire environment (choose Global | Save_current_environment pull-down menu item), and then you can simply re-load the environment to correct the R-T data.

A. Generate Corrected R-T data mode

The *Generate Corrected R-T Data* mode generates corrected R-T data from the baseline and sample measurements using Equation (3). It does not require any model for the sample at all; it only requires an accurate baseline model. The user can then save the corrected data, which is located in the Generated Data window.

A1. **Open the baseline reference sample model (or environment), if it is not already there.** This is the model (or environment) that was saved in section 0 above.

> 0 al_sub_2009-06-05_pbp_fit 1 mm

Figure 2. Model of Aluminum substrate reference sample, developed from analysis of reference sample ellipsometric data.

A2. **Open the sample reflectance data file** by selecting File|Open in the Experimental data window. This is the data that is going to be corrected.

A3. **Add the *rt_baseline.mat* to reference model** by Selecting AddLayer menu item, and add *rt_baseline.mat*. (This layer can

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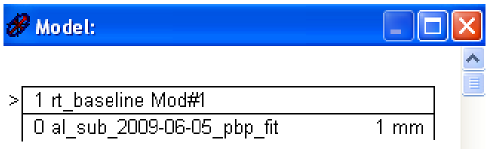
[4] To save a model, select the File|Save_model menu item in the Model window pull-down menus. Be sure to save any newly-created layers in the same directory as the model file, so that it is properly accessed in the next step.

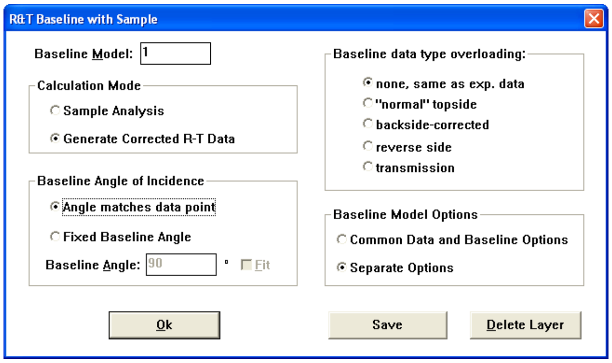


\> 1 rt_baseline Mod#1
0 al_sub_2009-06-05_pbp_fit 1 mm

Figure 3. Reference model after addition of rt_baseline layer.

A4. **Open the *rt_baseline layer* dialog box and select these options** (Figure 4).

- **Select 'Generate Corrected R-T Data' Calculation mode.**
- **Enter "1" in the Baseline Model box.** This value defines the model-window where the baseline model is located.
- **Select appropriate Baseline Angle of Incidence.** If the baseline and test sample were measured at the same angle, you can select 'Angle matches data point'. If the baseline angle was measured at a different angle than one or more of the test sample measurement angles, then select 'Fixed Baseline Angle' and enter the correct Baseline angle in the box. Under most circumstances, you will not want to fit the baseline angle of incidence.
- **Select the Baseline data type overloading.** In most cases, selecting 'none, same as exp. data' is appropriate, as the baseline and test sample data types are identical (i.e., pR, sR, etc.). An example where this would <u>not</u> be the case is the baseline is a transmission-type measurement, and the test sample is a reflection-type measurement.
- **Baseline Model Option**. *This option doesn't affect the results in the 'Generate Corrected R-T data' calculation mode.*



Baseline Model: 1

Calculation Mode
○ Sample Analysis
● Generate Corrected R-T Data

Baseline Angle of Incidence
● Angle matches data point
○ Fixed Baseline Angle
Baseline Angle: 90 ° ☐ Fit

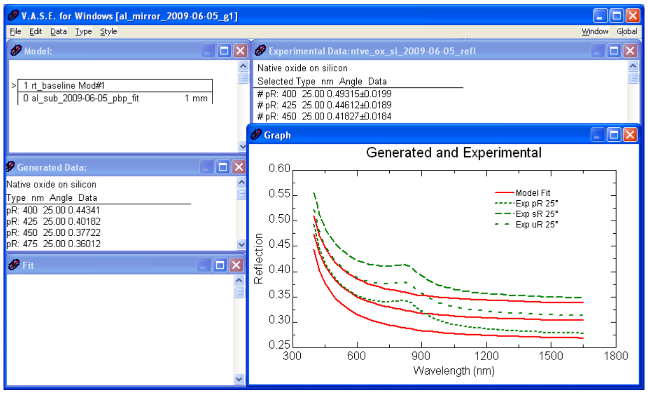
Baseline data type overloading:
● none, same as exp. data
○ "normal" topside
○ backside-corrected
○ reverse side
○ transmission

Baseline Model Options
○ Common Data and Baseline Options
● Separate Options

Figure 4. rt_baseline layer setup for generating Corrected R-T data.

A5. Generate Corrected R-T Data by selecting the Generate_Data menu item in the Generate Data window.

A6. Save Generated Corrected R-T Data by selecting File|Save_Gen._Data in the Generate Data window.



```
> 1 rt_baseline Mod#1
  0 al_sub_2009-06-05_pbp_fit          1 mm
```

```
Native oxide on silicon
Selected Type  nm  Angle  Data
# pR: 400  25.00 0.49315±0.0199
# pR: 425  25.00 0.44612±0.0189
# pR: 450  25.00 0.41827±0.0184
```

```
Native oxide on silicon
Type  nm  Angle  Data
pR: 400  25.00 0.44341
pR: 425  25.00 0.40182
pR: 450  25.00 0.37722
pR: 475  25.00 0.36012
```

Figure 5. WVASE® window after Corrected R-T data are generated. The corrected R-T data are are located in the Generated data window.

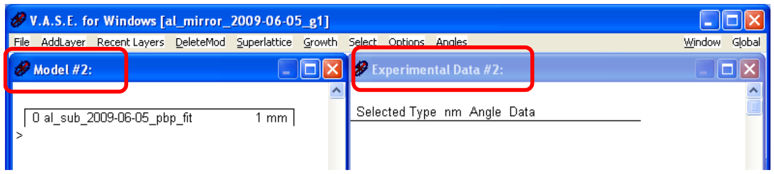
B. Sample analysis calculation mode

The “Sample Analysis” calculation mode allows the user to directly analyze the uncorrected R-T data from the test sample, without having to generate and save the corrected R-T data. In order to model the sample and fit the R-T data:

B1. Open baseline reference model into model-window #2. *We will reserve Model window #1 for modeling/analyzing the test sample*[5].

To accomplish this, first activate model-window #2 by selecting Alt–2. (You can also choose the ‘Select’ menu item in the Model window, then select current model #2 radio button). The Model and Experimental window title bars should have “#2”, as shown in Figure 6.

After model-window #2 is selected, load the baseline reference model (saved from step 0 above), by selecting ‘File|Open_model’ from the model window pull-down menus.



```
  0 al_sub_2009-06-05_pbp_fit          1 mm
>
```

```
Selected Type  nm  Angle  Data
```

Figure 6. Model Window #2. Various model windows can be accessed by selecting “Alt-1”, “Alt-2”, “Alt-3”, … “Alt-0”, or choosing the Select menu item in the Model Window.

B2. Create model of sample in Model-window #1 using the required layers, using the standard WVASE® model-building procedures.

1	sio2-thermal_ir-genosc	279.58 Å
0	silicon_ir-genosc	0.6 mm

Figure 7. Example of a model for the test sample, prior to the addition of the rt_baseline *layer.*

B3. Add the *rt_baseline.mat* to model-window #1 by Selecting AddLayer menu item, and add *rt_baseline.mat*. Thee model should look something like Figure 8. The “Sample Analysis” R-T data mode will function correctly regardless of where the *rt_baseline* layer is located in the model, with the exception of layer 0 (substrate).

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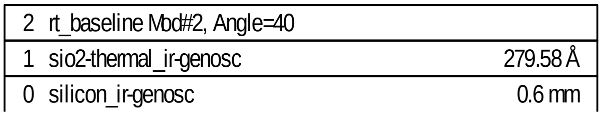
[5] For convenience and clarity of purpose, we reserve model-window #2 for the reference-sample optical model, and model-window #1 for the test sample and its data. Users can choose other model-window combinations to accomplish the same result.

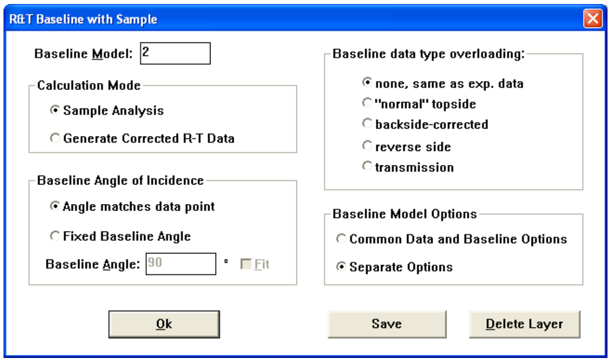


2	rt_baseline Mod#2, Angle=40	
1	sio2-thermal_ir-genosc	279.58 Å
0	silicon_ir-genosc	0.6 mm

Figure 8. Model for the test sample, after the addition of the rt_baseline *layer.*

B4. **Add the *rt_baseline.mat* to model-window #1** by Selecting AddLayer After the layer is added, select the following options from the *rt_baseline* layer dialog box (Figure 9).

- **Select 'Sample Analysis' Calculation mode.** This allows the user to directly analyze the uncorrected R-T data from the test sample, without having to generate and save the corrected R-T data.
- **Enter "2" in the Baseline Model box.** This value defines the model-window where the baseline model is located.
- **Select appropriate Baseline Angle of Incidence.** If the baseline and test sample were measured at the same angle, you can select 'Angle matches data point'. If the baseline angle was measured at a different angle than one or more of the test sample measurement angles, then select 'Fixed Baseline Angle' and enter the correct Baseline angle in the box. Under most circumstances, you will not want to fit the baseline angle of incidence.
- **Select the Baseline data type overloading.** In most cases the baseline and test sample data types are identical (i.e., pR, sR, etc.); therefore, select 'none, same as exp. data'. An example where this would not be the case is the baseline is a transmission-type measurement, and the test sample is a reflection-type measurement.
- **Select the appropriate Baseline Model Option.** *If you are using the 'Sample Analysis' calculation mode, the correct Baseline model option depends upon whether or not the sample model options are different than the baseline model.*



R&T Baseline with Sample

Baseline Model: 2

Calculation Mode
● Sample Analysis
○ Generate Corrected R-T Data

Baseline Angle of Incidence
● Angle matches data point
○ Fixed Baseline Angle
Baseline Angle: 90 ° ☐ Fit

Baseline data type overloading:
● none, same as exp. data
○ "normal" topside
○ backside-corrected
○ reverse side
○ transmission

Baseline Model Options
○ Common Data and Baseline Options
● Separate Options

Figure 9. rt_baseline layer setup for Sample Analysis.

The model is now ready for data fitting or any other data analysis tasks. Please note that you can append other data-types (such as ellipsometric data) to Model window #1. You can also add data and models to other model windows, with the exception of the model-window containing baseline reference sample model (model-window #2 in this example).