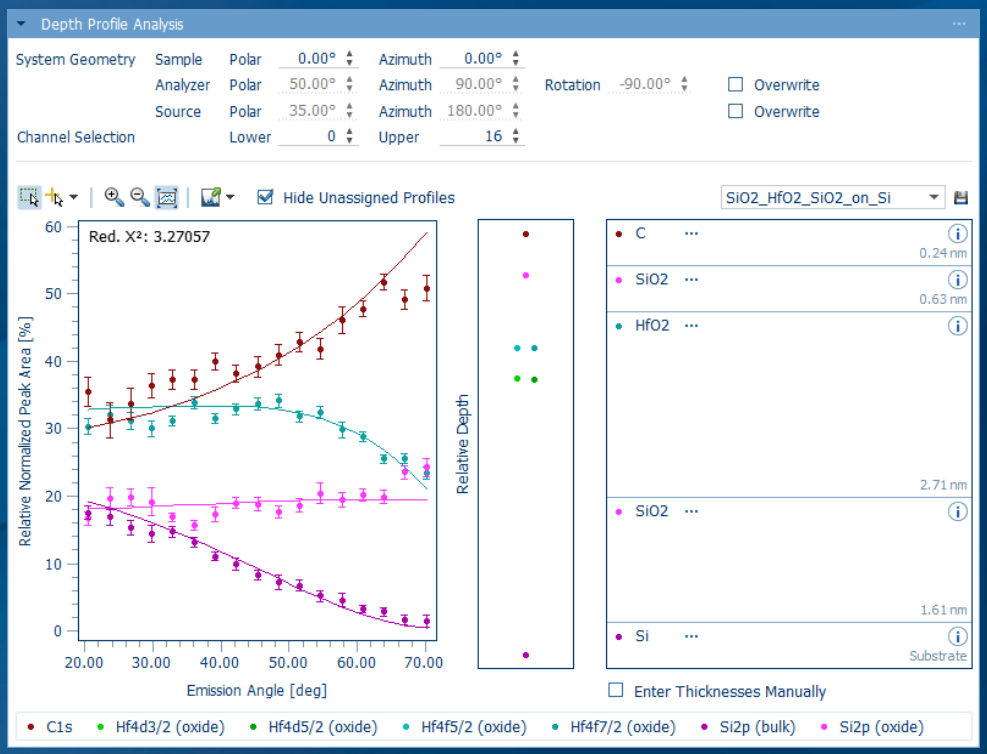
Prodigy ITFAP

Quick Guide to Identification of Thin Films From Angular Profiles



User Manual 4.103.1 | June 6, 2023

SPECS™

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SPECS User Manual

Prodigy ITFAP—Quick Guide to Identification of Thin Films From Angular Profiles
SpecsLab Prodigy Version 4.103.1

June 6, 2023

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Table of Contents

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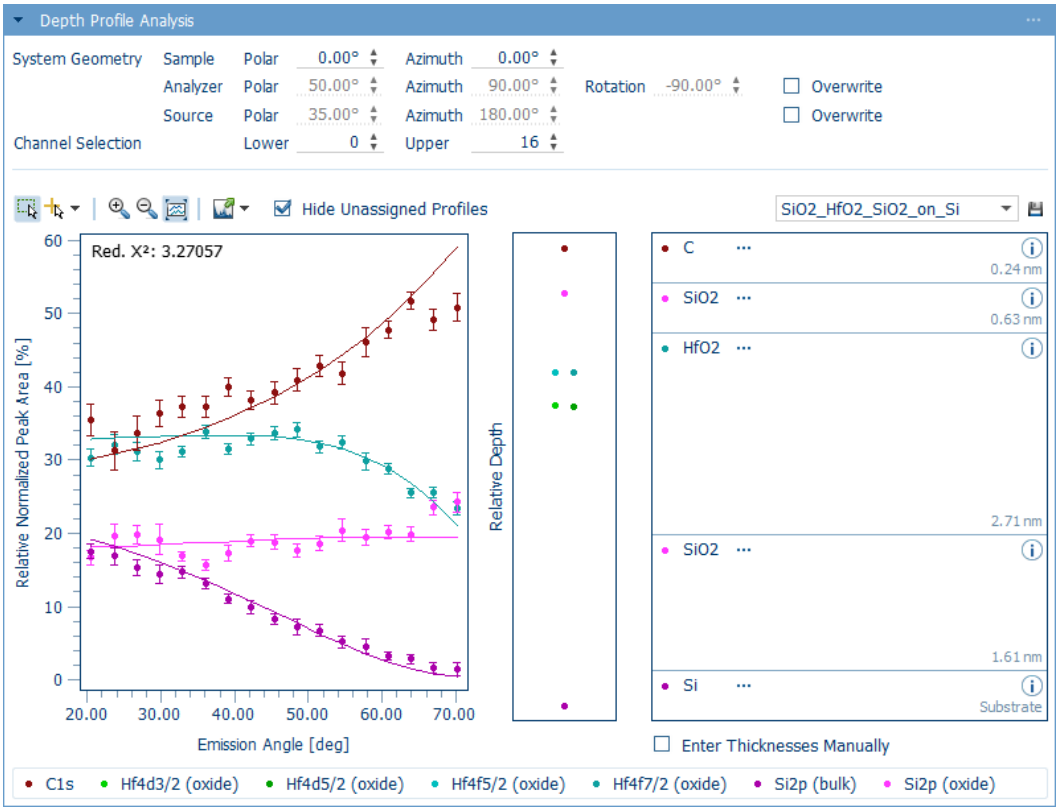
Chapter 1 – Overview

ITFAP is a software module integrated in SpecsLab Prodigy for non-destructive depth profile analysis of layered thin film samples by ARXPS.

1.1 User Interface

In SpecsLab Prodigy, the Depth Profile Analysis module appears with the interface shown below:



1.2 Key Features

The ITFAP module is a separately licensed option integrated with SpecsLab Prodigy. It compares angle profiles—peak areas as a function of emission angle—measured by parallel ARXPS and calculated for a layer model of the sample.

The following features are provided with ITFAP:

- Seamless integration with data acquisition
- Immediate layer structure information from relative depths of atomic species
- Easy input of proposed sample layer model
- Instantaneous optimization of sample model layer thicknesses
- Evaluation of consistency between sample model and ARXPS measurement via goodness of fit measure
- Quick comparison of sample models via sample model preset system
- Extensive parameter sourcing and control via SpecsLab Prodigy Chemical Databases

Chapter 2 – Prerequisites

2.1 General Information

The ITFAP module is recommended to users who have suitable experience in the field of ARXPS.

For advice and assistance, please contact SPECS support:

Tel. +49 30 46 78 24-0
email: support@specs.com

2.2 Configuration of System Geometry

Non-destructive depth profile analysis by ARXPS requires correct configuration of the system geometry. The SpecsLab Prodigy Configuration Tool is used to specify the orientation of

- analyzer, and
- X-ray source.

Both orientations are specified within a coordinate system attached to the analysis chamber (system coordinate system). For depth profile analysis, the orientation of the sample surface normal within the system coordinate system must also be specified. This is done during data analysis in ITFAP itself, not within the configuration tool.

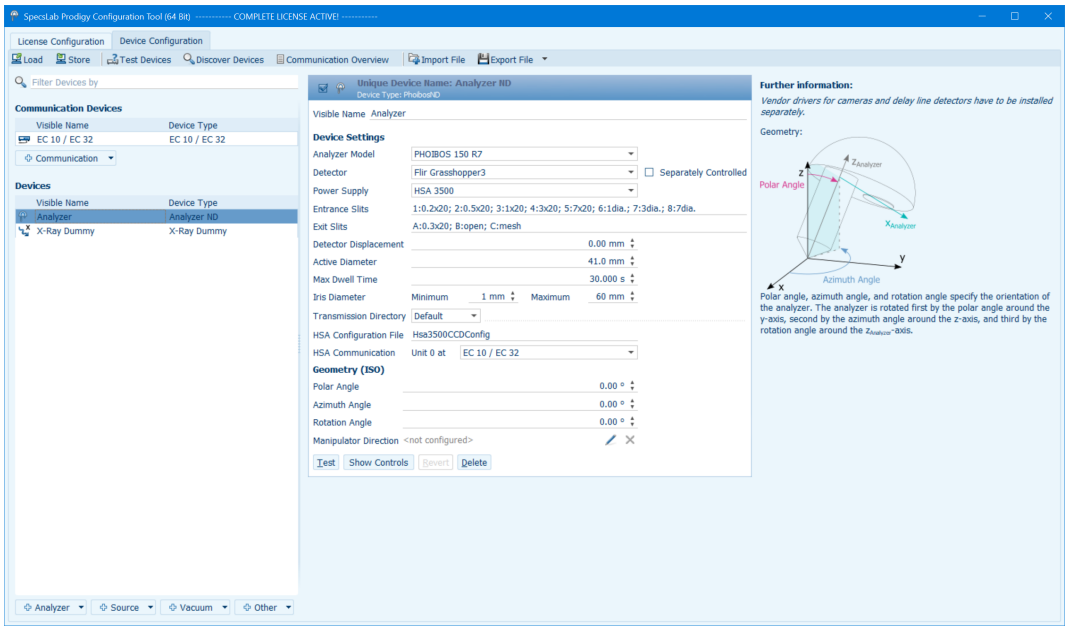
Note

It is possible to freely choose the orientation of the system coordinate system relative to the analysis chamber. Once this choice is made, it needs to be maintained when specifying the analyzer, source, and sample orientation.

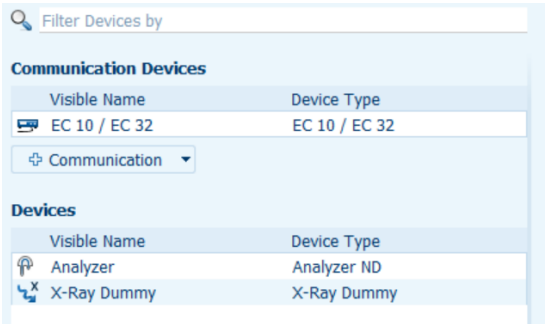
Often, the system coordinate system is chosen such that the sample surface plane lies within the x-y plane for a typical sample orientation.

To specify analyzer and source orientation, open the respective device configuration in the configuration tool and complete the steps described in the following paragraphs.

The figure below shows the analyzer device configuration:



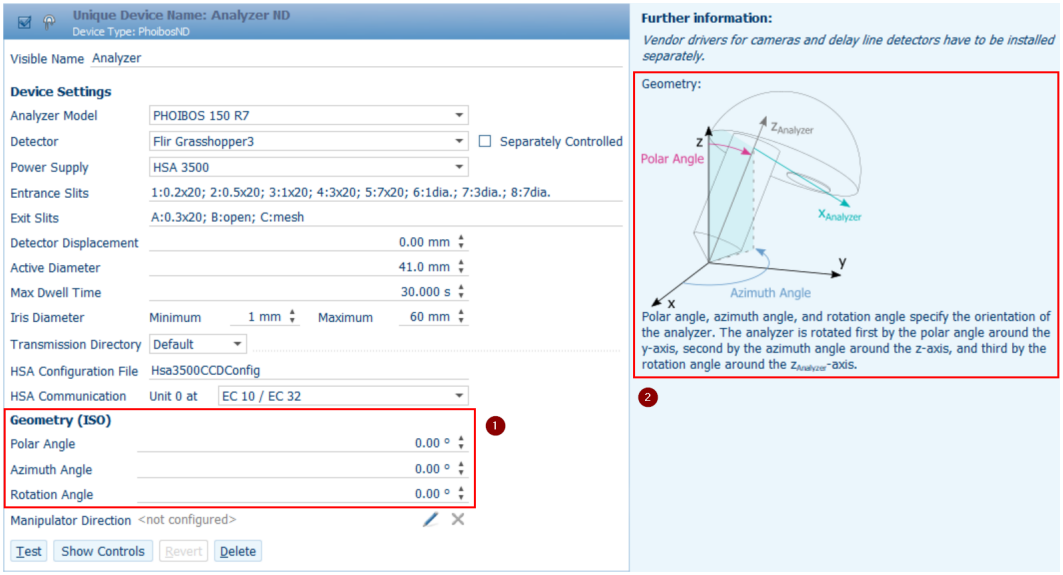
To access the source device configuration, switch from the analyzer to the X-ray source:



2.2.1 Orientation of the Analyzer

The below screen of the configuration tool shows the angular parameters (1) specifying the orientation of the analyzer with respect to the system coordinate system:

- *Polar Angle*
- *Azimuth Angle*
- *Rotation Angle*



The geometry sketch (2) in the image describes these parameters.

Coordinate Systems

In the above figure, the system coordinate system is colored black. It consists of the axes x, y, and z. The analyzer coordinate system consists of the axes

- $x_{Analyzer}$
- $y_{Analyzer}$
- $z_{Analyzer}$

The analyzer coordinate system is a right-handed coordinate system, where $z_{Analyzer}$ is the optical axis of the analyzer lens and $x_{Analyzer}$ points in the direction of increasing electron kinetic energy on the detector.

How to Specify the Analyzer Orientation

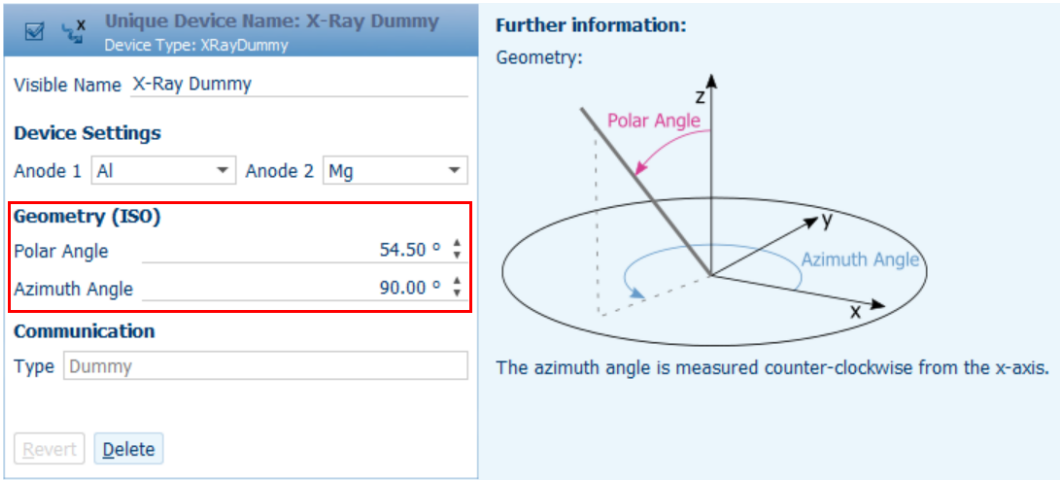
Starting from a situation where the analyzer and system coordinate system are congruent, the analyzer orientation results from the following successive right-handed rotations:

1. Rotation of the analyzer by the *Polar angle* around the y-axis.
2. Rotation of the analyzer by the *Azimuth angle* around the z-axis.
3. Rotation of the analyzer by the *Rotation angle* around the $z_{Analyzer}$-axis.

2.2.2 Orientation of the X-ray Source

In the Configuration Tool, the source orientation is specified with respect to the system coordinate system using the angular parameters:

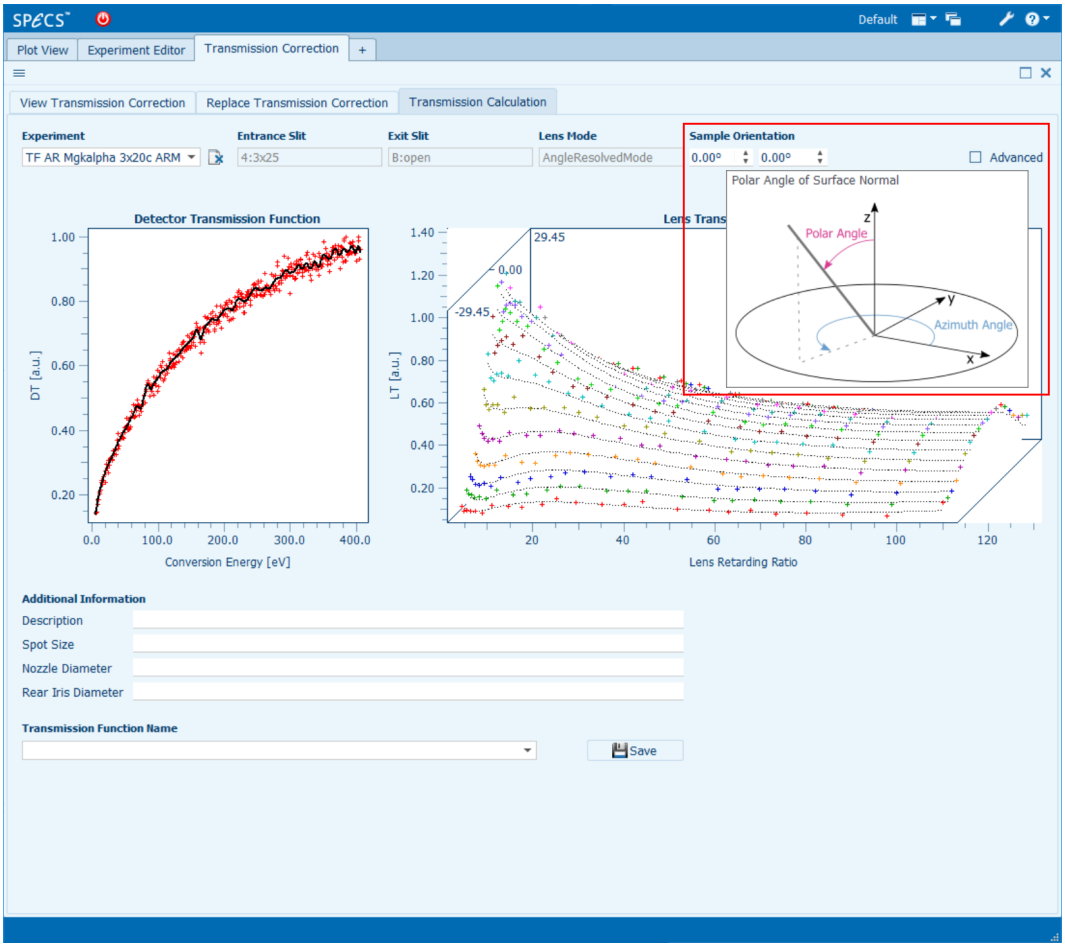
- *Polar Angle*
- *Azimuth Angle*



These parameters define the direction of the beam axis within the system coordinate system.

2.3 Angle-resolved Transmission Function

It is recommended to measure an angle-resolved transmission function specific to the geometry used for ARXPS data acquisition:



In SpecsLab Prodigy's *Transmission Correction* view, the orientation of the sample surface normal is specified via its polar and azimuth angle with respect to the system coordinate system. The analyzer and source orientation are used as specified in the configuration tool.

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Chapter 3 – ARXPS Depth Profile Analysis

Non-destructive depth profile analysis is perfomed in the following steps:

- Measurement of detailed angle-resolved XPS spectra
- Peak fitting
- Depth profile analysis within ITFAP

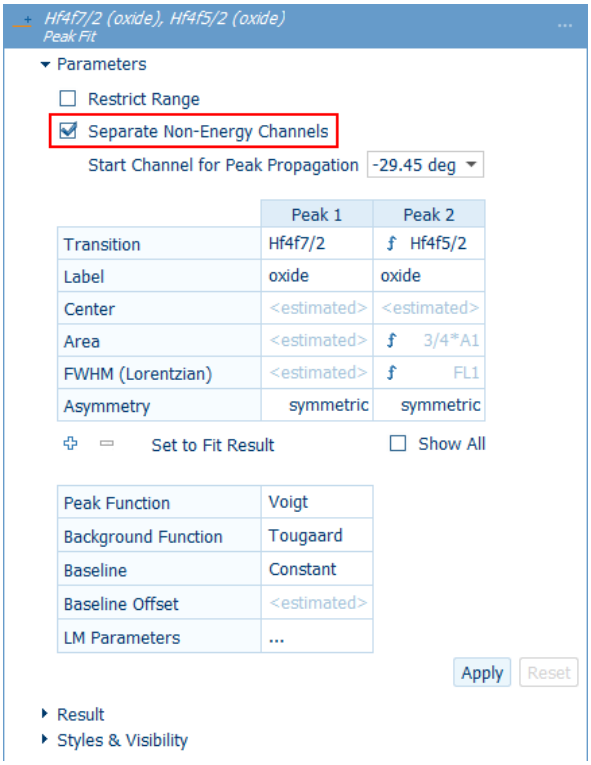
These steps are described in more detail below.

3.1 Measurement of Detailed Angle-resolved XPS Spectra

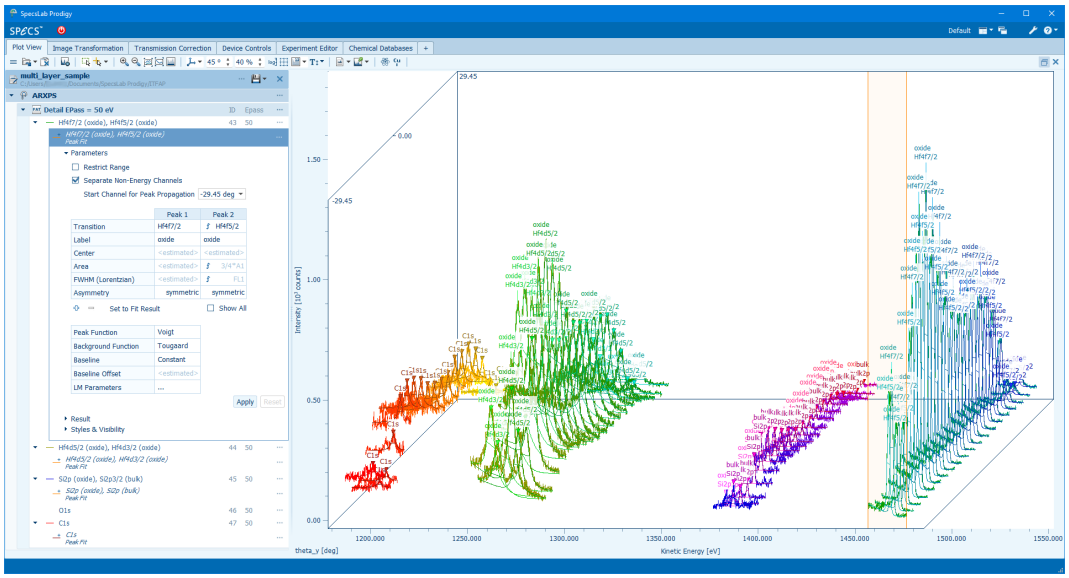
In the first step, acquire detailed ARXPS spectra with the peaks of the atomic species to be considered for depth profile analysis. Use an angle-resolved transmission function for the given sample position and orientation.

3.2 Peak Fitting

Fit the peaks, separating the angular channels of the spectrometer.

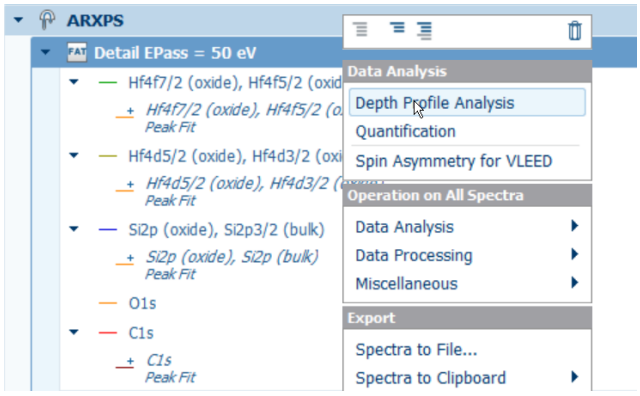


SpecsLab Prodigy's *Peak Fit* operation automatically propagates peak function parameters starting from a user-selectable start channel.

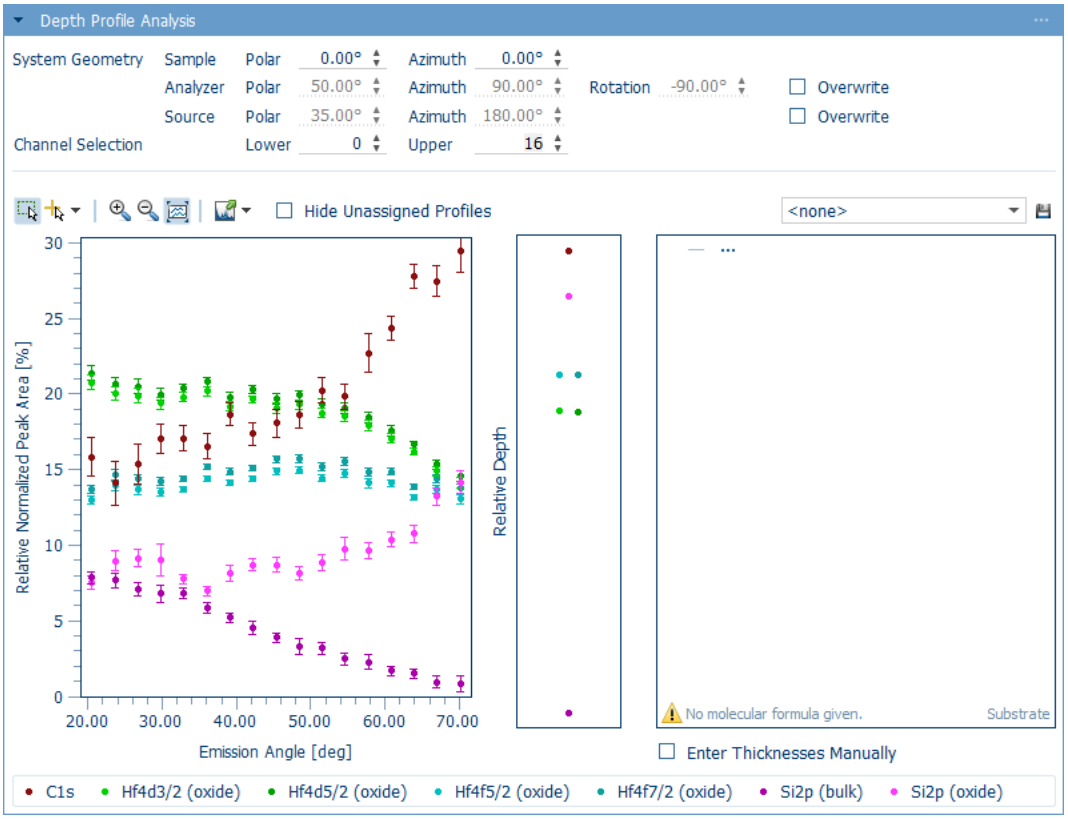


3.3 Depth Profile Analysis

Apply a *Depth Profile Analysis* operation on the spectrum group.



The angular profiles and relative depths are available immediately in *Depth Profile Analysis*:

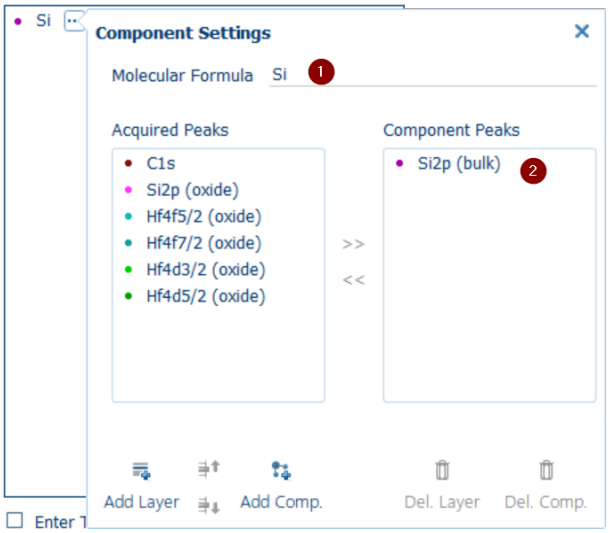


3.4 Sample Model Definition

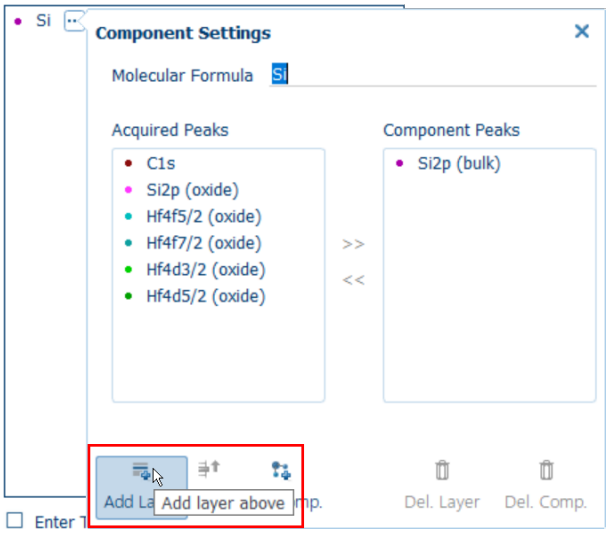
The next step is to define the sample model based on the relative depths and known sample properties. For this purpose, the sample model editor is used.

To specify the substrate composition, open *Component Settings* by clicking here:

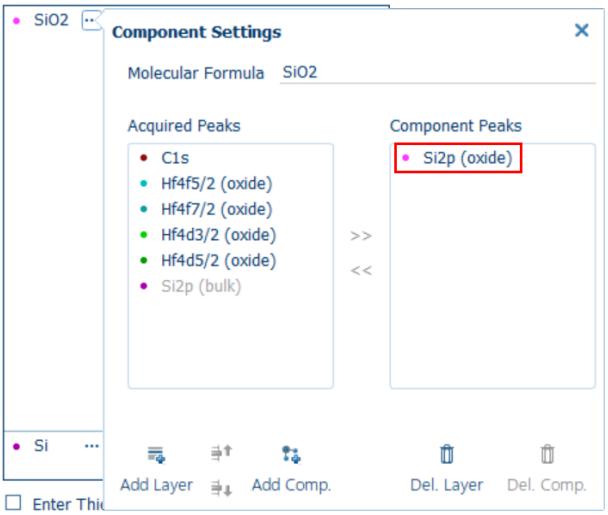
Enter a molecular formula (1) and assign peaks to the component (2):



Add layers above the substrate ...



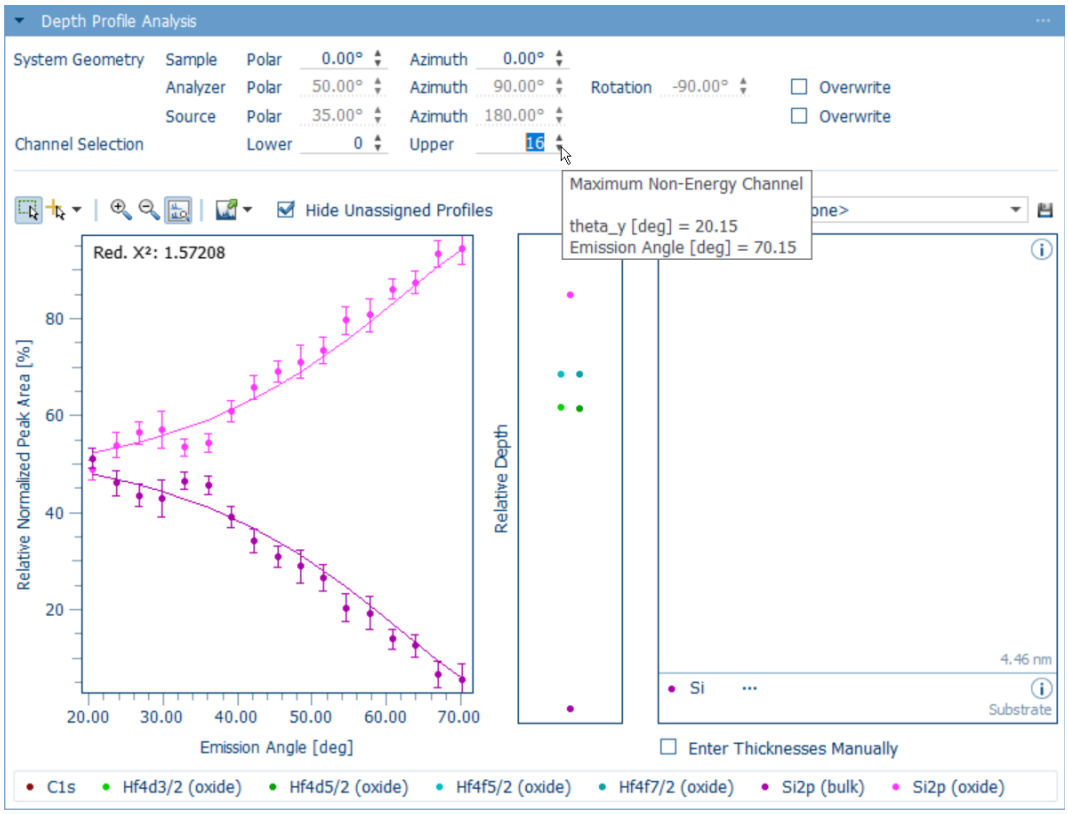
... and specify their components:



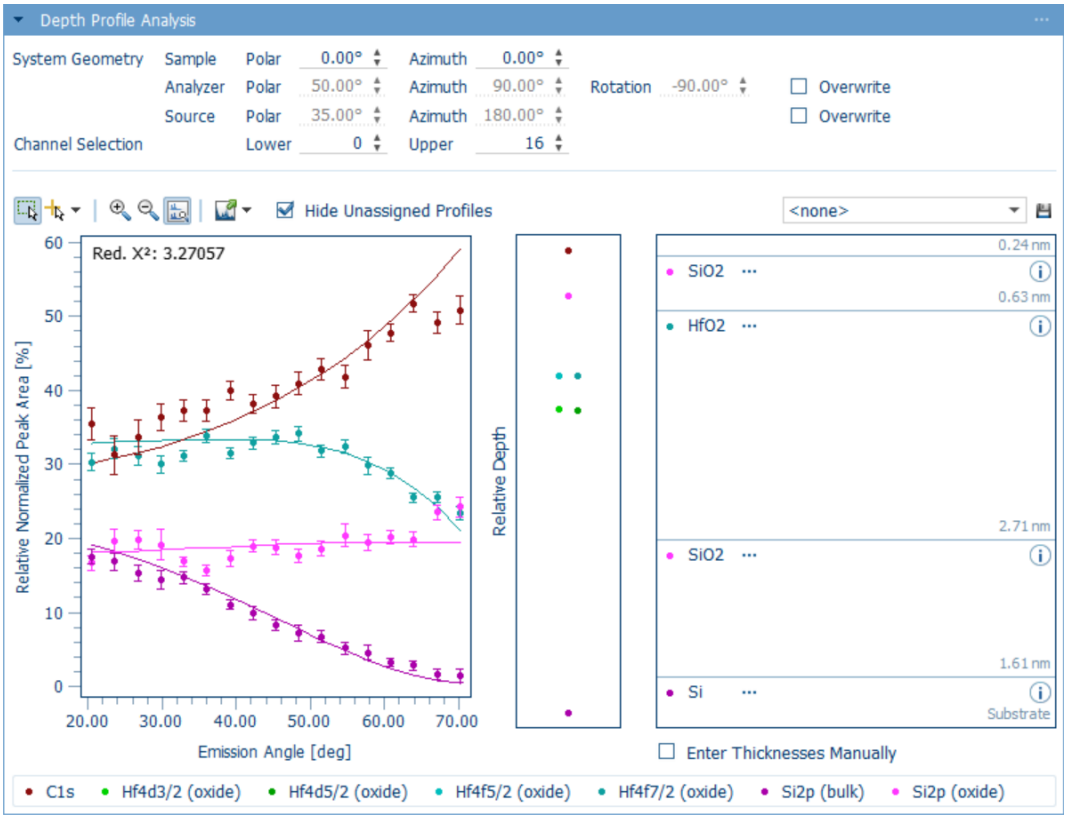
For the sample model given, angle profiles are calculated immediately. The layer thickness is optimized for best fit of the calculated angle profiles to the measured angle profiles.

Angle profiles are only calculated for peaks assigned to components of the sample model. A comparison of *relative* calculated and measured angle profiles requires only those measured profiles to be considered, for which also a calculated profile exists. Check *Hide Unassigned Profiles* to exclude measured profiles without a calculated counterpart.

In the example used, relatively high uncertainty of the peak areas is apparent at the largest emission angles. These peak areas can be excluded from the fit by using the upper *Channel Selection* limit:

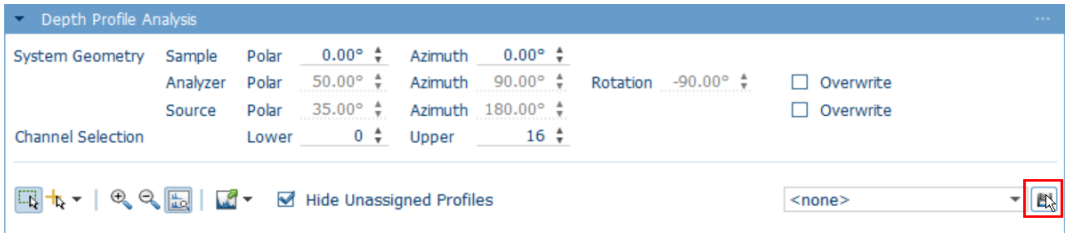


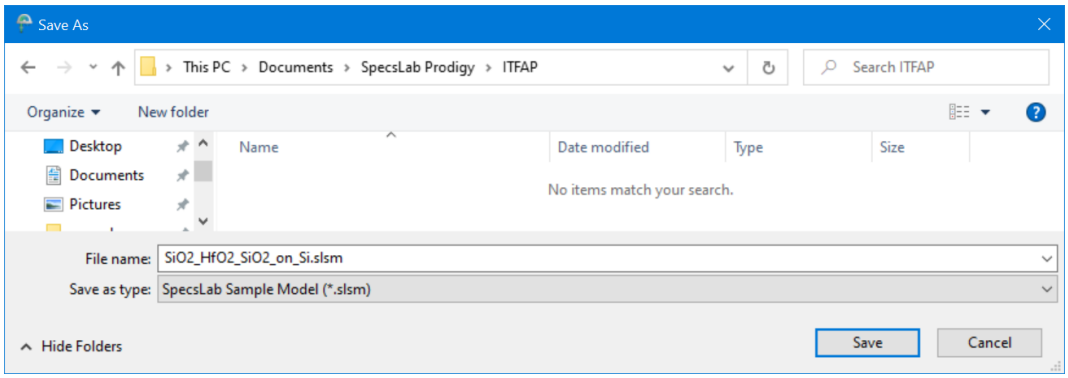
In the way described, more layers can be added in order to model the expected sample structure. Upon definition of a new layer, layer thicknesses are instantly optimized for the layer sequence defined. A reduced chi-squared (Red. X^2) is calculated as a measure of goodness of fit:

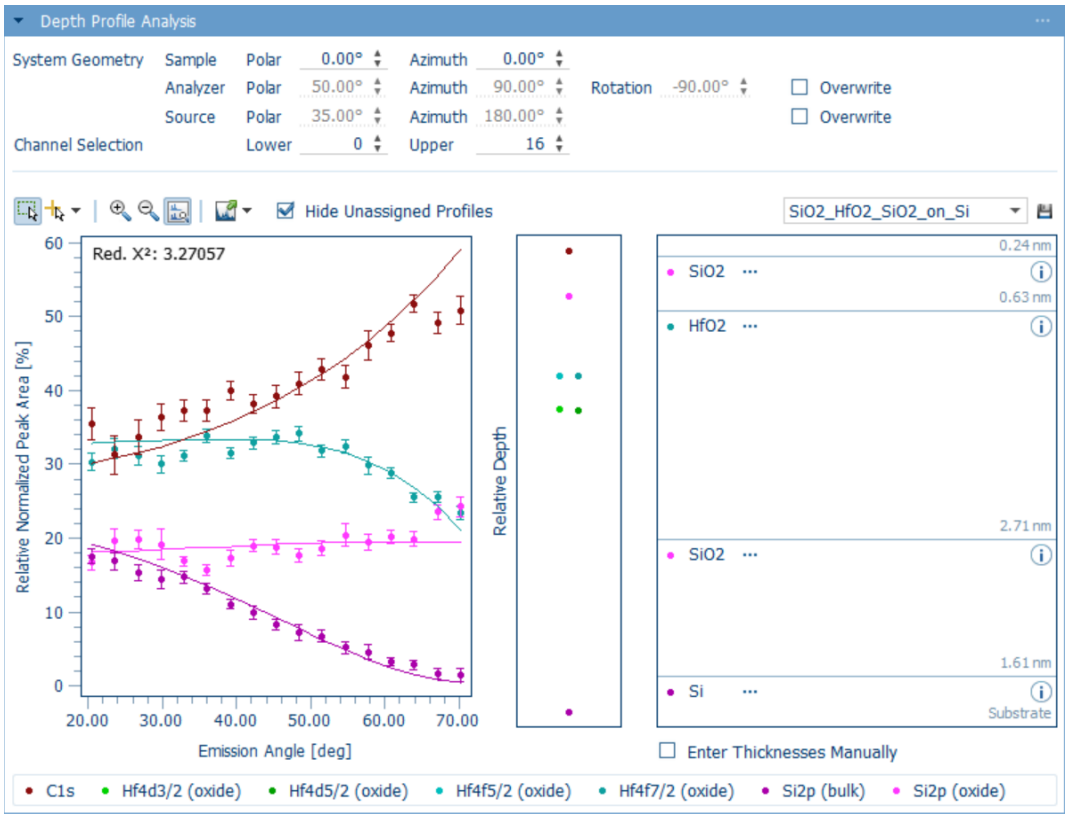


3.5 Sample Model Presets

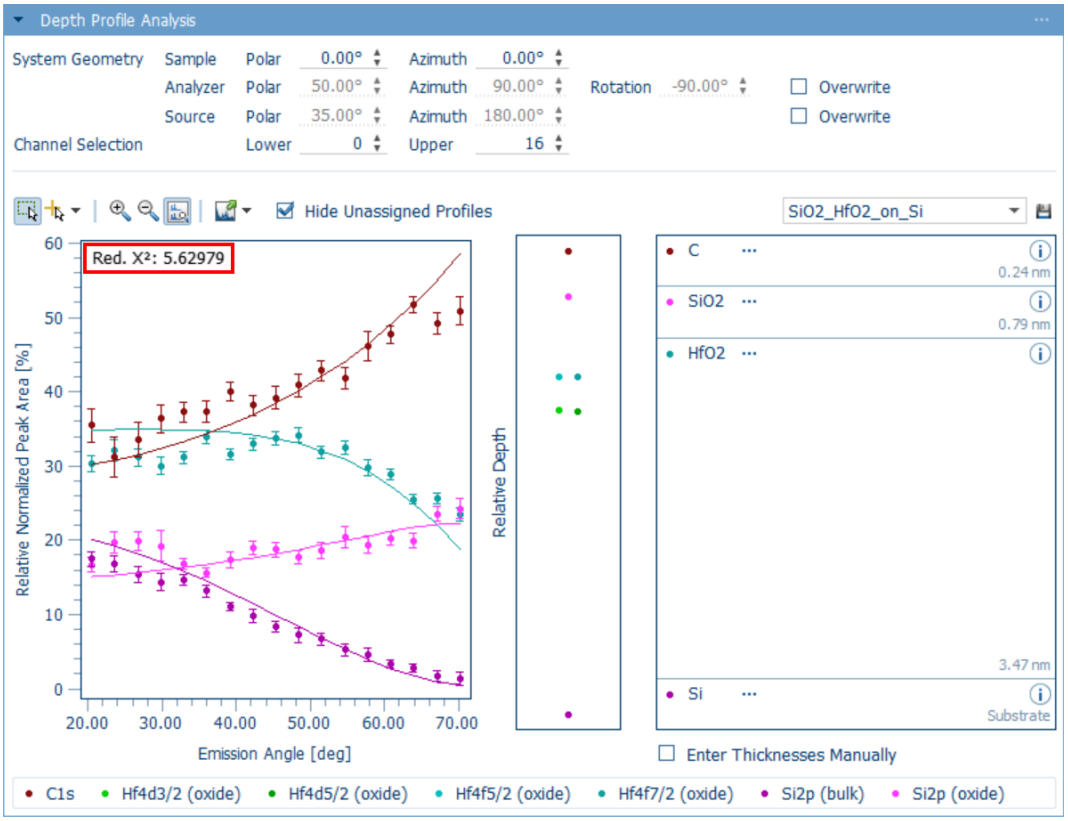
Sample models can be stored as presets:







Presets make comparison of different sample models particularly easy. In the screenshot below, a preset was loaded, where the sample model does not comprise an oxide layer on the silicon substrate. The larger resulting chi-squared shows immediately, that omitting the oxide layer reduces fit quality:



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