SpectraRay/3
Software for spectroscopic ellipsometry

Product description

1 General description

SpectraRay/3 is SENTECH’s comprehensive software for spectroscopic ellipsometry. It is shipped with all spectroscopic ellipsometers and is available as standalone version.

SpectraRay/3 provides a user friendly workflow oriented user interface to operate SENTECH’s spectroscopic ellipsometers and a comprehensive set of tools to model, to fit and to represent ellipsometric data. The user interface incorporates a recipe oriented operation for operators and an advanced mode for interactive measurement and modeling. The advanced mode is intended for process engineers or research applications.

SpectraRay/3 allows to measure:

- Film thickness
- Thickness of each layer in a layer stack (number of films no restricted)
- Refractive index and absorption index (extinction coefficient) of materials, films and layer stacks (dispersion)
- Reflection ($R_s$, $R_p$, $R_{cross}$, $R$) and transmission ($T$)
- Composition of materials (e.g. alloys)
- Vertical changes in optical constants (non-uniformity of materials, index gradient)
- Thickness of interfaces, surface roughness (e.g. mean thickness of rough surface layer)
- Generalized Ellipsometry: Anisotropy of materials, films and layer stacks (uniaxial and biaxial), handles non-diagonal elements of the Jones Matrix of the sample
- Mueller-Matrix measurements (12 elements with single retarder or 16 elements with dual retarder)
- Incoherent calculation for modeling thick substrates (compared to coherence length of light)
- Fundamental gap of materials (e.g. semiconductors, dielectrics, metal oxides)
- Plasma frequency
- Concentration and mobility of charge carriers, conductivity
- Oscillator frequency, oscillator strength and damping factor of molecule vibrations
- Growth rate and type of growth of films
SpectraRay/3 supports variable angle, multi-experiment and combined photometric measurements (ellipsometric, reflection and transmission measurements).

**Generalized ellipsometry** supports the measurement and theoretical handling of anisotropic samples (layer stacks or nanostructured wafers). It measures the non-diagonal elements of the Jones matrix of such samples in addition to the measurement of isotropic samples.

**Mueller matrix measurements** are supported and measure the response of a sample to incoming polarized light in a most general way. Twelve elements of the Mueller matrix are measured with (PCSA\(^1\) and PSCA) setups like the SENresearch ellipsometer. The PCSCA setup allows the measurement all 16 elements.

SpectraRay/3 includes a huge library of materials data based on SENTECH’s measurements and literature data as well. The large number of dispersion relations available in SpectraRay/3 allows modeling any type of material under investigation nowadays.

SpectraRay/3 measures uniaxial and biaxial anisotropic materials, films, and layer stacks on any type of substrate including incoherent calculation of beam overlay.

SpectraRay/3 includes all utilities of general spectroscopic software package for data import and export (ASCII included), file management, arithmetic manipulations of spectra, display, printing and reporting (in Word file format *.doc).

SpectraRay/3 includes a macro language for user defined tasks (scripting). It can be operated in an **Interactive Mode** which is preferred especially for usage in research (e.g. running complex measurement tasks, export or import of data in Excel spreadsheets). The Interactive mode allows access to all features of SpectraRay/3. Another application of the scripting engine is to connect to other hardware and software and to incorporate this into the measurement sequence.

SENTECH offers special application scripts for push button operation especially useful for routine work such as data monitoring and quality control in a production environment.

SpectraRay/3 requires Windows XP, Windows Vista or Windows 7 as operating system (both x86 and x64 versions are supported). At the time of writing ellipsometer devices are shipped with x86 versions of Windows 7 (others on request). For standalone versions there is preference either for x86 or x64 versions of Windows.

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\(^1\) Setup principle with component list from source to detector (P-polarizer, C-retarder, S-sample, A-Analyzer)
2 SpectraRay/3 software in glance

Main operation window of SpectraRay/3: interactive mode
Data acquisition
Modeling
Modeling: Dispersion model Tauc-Lorentz

![Image of Dispersion model Tauc-Lorentz]
Fitting: Measured and fitted spectra
Reports in Word format
3 Specifications

3.1 Data analysis:

- Variable angle measurements,
- Mueller matrix measurement (12 elements with PCSA and PSCA setups, 16 elements with PCSCA setups)
- Generalized ellipsometry (Anisotropy): The data acquisition supports the sample orientation entered manually as well as automatic measurements using a rotation stage
- Multiple experiments (e.g. samples with similar optical properties but different film thickness)
- Combined photometric measurements ($\Psi$, $\Delta$, $R$, $R_p$, $R_s$, $R_{cross}$, $T$)
- Transparent samples with backside correction

Software correction of backside reflection

3.2 Modeling

Model options:

- Substrate (material)
- Single film on substrate
- Multiple layer stack (number of layers not restricted)
- Multiple model to fit different samples and photonic data ($\Psi$, $\Delta$, $\phi$, $T$, $R$) together
- Consideration of depolarization effects
- Transparent samples, modeling of backside effect

2 The automatic rotation stage is optional hardware, SpectraRay uses it if present.
Materials library:
- More than 200 material data for dielectrics, semiconductors, metals and organic materials like polymers available.

Sample Library:
- More than 100 sample experiments as a starting point for learning modeling.

Layer types, dispersion models:
- File layer (look up table data)
- Dispersion models for uniform films and materials

- Cauchy, Schott, Sellmeier, Urbach, Drude-Lorentz, Tauc-Lorentz, Leng, Sernelius, Hambach, Brendel, Tanguy, Afromowitz, Forouhi Bloomer, Anisotropy (biaxial and uniaxial), Nuclei growth, User defined function

- Alloys and composites (Effective medium approximation)
  - Bruggeman model,
  - Maxwell-Garnett model
  - Chemical mixture

- Periodic layer structures (superlattices)
- Rough surfaces and interfaces
- Index gradients (linear, Gaussian, exponential function, error function, arctan-function)
Vertical gradient of refractive index of ITO film described by EMA model (Bruggeman)

3.3 Fitting

- Very fast fitting algorithms
- Thickness scan
- Fit stop control
- Data selection
- Parameter scanner for manual and automated adjustment of fit parameters

The fitting procedure is accompanied by a utility to evaluate the quality of the optical model compared to the current measurement. This allows the detection of over determined optical models and evaluates the effective accuracies and gives hints on improving the model.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
<th>Refractive Index</th>
<th>Absorption</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>0.16 nm</td>
<td>1.0000</td>
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</tr>
<tr>
<td>SiO2</td>
<td>4.28 +/- 0.1 nm</td>
<td>1.4510</td>
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<tr>
<td>p+aSi</td>
<td>53.6 +/- 0.2 nm</td>
<td>3.6618 +/- 0.0096</td>
<td>0.0598 +/- 0.0038</td>
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<tr>
<td>Corning glass</td>
<td>1.5087</td>
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<td>0</td>
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</table>
Scanner: Search for starting parameter of film thickness
4 Statistics

- Mean error, standard deviation, correlation matrix

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<tr>
<th>Name</th>
<th>Fit</th>
<th>Value</th>
<th>Error</th>
<th>[1.1] roughness - EMA - Thickness [nm]</th>
<th>[92] roughness - EMA - Thickness [mm]</th>
<th>TIO2 - TL Eq(1)</th>
<th>TIO2 - TL Eq(2)</th>
<th>TIO2 - TL Eq(3)</th>
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<tbody>
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<td>[1.1] roughness - EMA - Thickness</td>
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<td>8.16</td>
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</table>

5 Reporting

- Copy data and spectra to clipboard for using in different text and graphic processors
- Extended reporting function for graphics and data
- Printing
- Editable reports in Word format (*.doc)

Software window to organize the reporting of data and spectra
6 Scripting

- Macro language to develop user defined measure and operation routines
- Push button applications
- Customize reporting (report generation is done by script and this allows to change the style) and templates (you may have any number of report elements which can be changed in a sequence)
- Load and save data in a variety of formats (*.txt, *.spc, *.xls and more)
- Use network connectivity with other software (you may drive the whole software remotely from programs like Excel (use Visual Basic) or even Labview (use Labview ActiveX interface)

Script editor in use to customize the reports