



Manual of kSEMAW 0.9.6 software

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1 What kSEMAW can do

kSEMAW (Spectro-Ellipsometric Measurement Analysis Workbench) is a workspace for the analysis of Spectrophotometric (SP), Ellipsometric (ELI) and Photothermal Deflection Spectroscopy (PDS) measurements. The letter “k” indicates the use of the Qt libraries to generate the graphical user interface, typical of the desktop Linux KDE environment. kSEMAW allows to:

1. simulate SP, ELI and PDS measurements of a multilayer structure, knowing the thicknesses and the complex refractive indexes $\tilde{n} = n - ik$ of each material composing the different layers¹;
2. calculate the complex refractive index $n - ik$ and the thickness of a given layer (if “thin”) from experimental measurements (SP, ELI, PDS), knowing the thicknesses and the complex refractive indexes of all the other layers composing the structure;
3. evaluate the mean value of physical quantities (for example transmittance or reflectance), weighted on a given international standard spectrum (such as the illuminant D65 or the direct solar spectrum ASTM G173-03) or on a customized reference spectrum (for example the crystal scintillator PbWO₄ luminescence spectrum, used in the CMS experiment at CERN LHC);
4. predict reflectance/transmittance angular trends, once the realistic model of the coating has been set or by means of the equivalent model algorithm [1]; where necessary output spectra can be weighted over a given reference spectrum.

From version 0.8.0 onwards, the calculation of the near-specular solar-reflectance as a function of the acceptance angle (mirrors for Concentrated Solar Power) has been removed, because the new software SMQexpo, specific for solar mirrors, equipped with a more advanced equivalent model, is now available. Such software embraces the Open Source philosophy and is freely distributed; interested people can request it by sending an email to marco.montecchi@enea.it.

kSEMAW uses a mathematical approach based on transfer matrices, particularly suitable for the case of multilayers: in addition to being able to treat coherent propagation and interference (for arbitrary incidence angles), it also allows to simulate the effects due to different types of non-ideal material properties, such as optical constants gradients along the film thickness, thickness inhomogeneity, porosity and roughness. The latter is modelled by assuming the thickness to be Gaussian-like distributed with standard deviation σ , and variations along distances much greater than the wavelength λ . The program deals with moderately rough interfaces ($\sigma \ll \lambda$) and limited radiation diffusion [2].

kSEMAW can model devices composed by up to 9 layers of different materials. For each layer it is possible to: i) consider it as optically *thin* or *thick* with respect to the radiation coherence length², for summing up coherently or not the contributes originating from its two interfaces in wave propagation; ii) set a refractive index profile along the thickness; iii) introduce roughness at the outermost interface; iv) consider the layer as

¹kSEMAW adopts the convention of negative sign for the imaginary part of both the complex refractive index and dielectric constant; this convention derives from considering the plane wave solution of the Maxwell equations with positive time expressed as $\exp[i(\omega t - \mathbf{q} \cdot \mathbf{r})]$.

²According to the Heisenberg uncertainty principle the coherence length is $\Delta l \sim \frac{1}{2\pi} \frac{\lambda^2}{\Delta \lambda}$ where $\Delta \lambda$ is the radiation band-width.

composed of a mixture of two different materials with optical constants calculated on the basis of the Effective Medium Approximation method. The latter feature can be used to model porosity, by considering the layer as composed by a mixture of material and voids (air) in a given percentage.

To obtain the unknown n and k values of a film starting from experimental measurements kSEMAW uses two different methods:

- **solution-tracking search method;**
- **hybrid computational method, called “IbridOne”.**

Solution-tracking search method

The first step of the solution-tracking method is to search for a (n, k) couple of values that reproduces the experimental measurements at a given λ (typically λ_{min} and λ_{max} of the considered wavelength range). The search is separately performed for each experimental measurement within the region of the (n, k) space chosen by the user: the n -interval is sampled with 51 points and, for each one of them, the k value which reproduces the experimental data is found by means of a bisection method; then a similar procedure is repeated by exchanging n with k . All these results are graphically displayed by drawing the solution-belt in the (n, k) space, where the width of the belt is determined by the experimental error.

To ensure good accuracy it is necessary to choose at least a couple of measurements M_1 & M_2 (like T & R or Δ & Ψ) that gives rise to solution-belts almost orthogonal one to the other: their cross-section contains the wanted common (n, k) -solution of the two or more considered measurements; sometimes multiple crossings are present. In any case the user is asked to select the more appropriate initial values at λ_{min} and/or λ_{max} .

Once the initial values have been set, the user can launch the tracking method: starting from the minimum or maximum wavelength the solutions n_λ and k_λ of the following wavelength are numerically computed by minimizing the merit function $MF = \sum_i (M_{i,cal}(n, k) - M_{i,exp})^2 / \Delta M_i^2$. The process is sequentially run over all the wavelengths sampling the wavelength range.

As the search progresses, the solutions n_λ and k_λ are plotted in two dedicated windows describing a portion of the spaces (λ, n) and (λ, k) . At the end of the process, by observing the set of solutions in the (λ, n) space, one can note that zero, one or more solutions can exist for each wavelength in the case of a thin film; in addition, the set of solutions is not necessarily connected. By optimizing the model parameters (thicknesses, roughness, gradients, etc.) according to specific guiding criteria [3, 4], a more connected set of solutions can be obtained; finally, among them, a physically reasonable subset of solutions must be selected.

HybridOne computational method

In the IbridOne method:

1. $n(\lambda)$ is modelled with appropriate analytical functions described in detail in Appendix A;
2. the extinction coefficient $k(\lambda)$ is numerically computed from $T(\lambda)$ and the assumed $n(\lambda)$;

3. the computed reflectance $R_{comp}(\lambda)$ is compared with the experimental one by means of a merit function;
4. some parameters of the assumed $n(\lambda)$ analytical function as well as of the optical model are optimized by a non-linear least square algorithm.

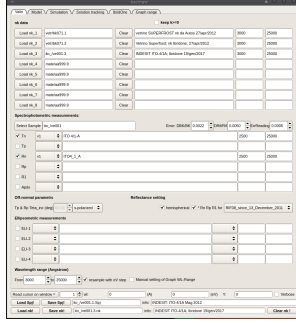
Before starting the optimization with the IbridOne method, the function parameters have to be set to initial values good enough to reasonably model $n(\lambda)$. Then, assuming $n(\lambda)$, $k(\lambda)$ values are calculated to perfectly reproduce the spectrum $T(\lambda)$; from the knowledge of $n(\lambda)$ and $k(\lambda)$, the reflectance spectrum $R_{cal}(\lambda)$ and the merit function $\chi^2 = \sum_i (R_{cal}(\lambda_i) - R_{exp}(\lambda_i))^2 / \Delta R_i^2$ are calculated. The Levenberg Marquardt non-linear least squares curve fitting (offered by the MINPACK library) is then used to minimize χ^2 optimizing some parameters of the coating model (e.g. thickness) and of the analytical functions used to describe $n(\lambda)$. Note that when using IbridOne the transmittance spectrum is always perfectly reproduced by construction.

In order to choose the most appropriate analytical functions to be used in IbridOne, at least in the initial phase, it is advisable to launch the tracking method first, to identify the wavelength-behaviour of a physically meaningful solution subset. Otherwise, the choice of oscillator functions should be driven by the physical properties of the material under investigation: in this case the oscillator parameters in the Simulation TAB has to be manually adjusted to obtain a first rough reproduction of the experimental curve before launching IbridOne.

In any case, users should never forget that the reliability of the obtained n, k solutions strictly depends on the correctness of the experimental measurements used as input data.

Appendix B reports some rules of good practice to avoid the most common coarse errors causing artefacts in spectrophotometric measurements.

GUI based on Qt and C++
ksemaw executable



write command

text file
ksemaw.ctrl

write parameters

text file
defau.1.Spj

if != "p"

run job

FORTRAN written
ksemawf executable
running in background

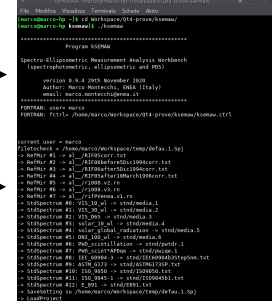


Figure 1: Workflow at the launch of a given command from the kSEMAW GUI.

2 Computer notes

kSEMAW consists of two executables. The first, named **ksemaw**, C++ written, and based on Qt libraries, manages the graphical user interface (GUI) for data input-output. The second one, named **ksemawf**, FORTRAN written, runs in background and executes the required computing.

The two executables interact by means of the two text files **ksemaw.ctrl** and **defau.1.Spj**:

the former contains the imparted command or the process status, the latter the full parameter set characterizing the current project. Figure 1 describes the workflow at the launch of a given command from the GUI. Once the imparted task has been completed, the FORTRAN executable writes “p” in the file **ksemaw.ctrl**; the executable C++, alerted by the modification of that file, once found “p”, reloads **defau.1.Spj** which in the meanwhile has been refreshed by **ksemawf**.

Two different ways for installing kSEMAW are available: i) compilation of source files; ii) installation of a virtual machine where kSEMAW has been pre-installed. Code source files, user manual as well as a sample of working directories populated with assorted files can be freely downloaded from <https://sourceforge.net/projects/ksemaw/>. Concerning the pre-configured virtual machine, please contact the corresponding author.

2.1 Source file compilation in Linux operative systems

The compilation in OS other than Linux is not here presented. For Microsoft Windows users a very interesting option is the Linux installation in dual-boot: at booting a “grub” menu will pop-up, allowing the user to choose the OS to be used.

The installation from source files described in the following requires at least a basic knowledge of Linux operative systems. After the installation of his own favourite Linux distro, the user has to install Qt and pgplot libraries; conversely a customized version of MINPACK is directly included in the source files.

The FORTRAN executable is built with the script `semaw.shcf` which compiles all `*.f` source file. Finally the commands `qmake` & `make` launch the compilation of the `*.cpp` source files getting the executable C++.

In the following more details of the installation in Linux distro based on Ubuntu are given.

Once Linux runs, the installation steps are:

- a. before installing new packages, one should update the whole system by typing in a terminal the commands

```
sudo apt-get update
sudo apt-get dist-upgrade
```

(in the case of error, `sudo dpkg --configure -a` followed by `sudo apt-get install -f`, and then `dist-upgrade`) and finally re-boot. Alternatively one can directly use the update manager by clicking on the small shield icon on the right of the bottom panel.

- b. with the refreshed system, installation of the compilers `gcc g++ gfortran`

```
sudo apt-get install gcc g++ gfortran
```

- c. library installation

```
sudo apt-get install qt5-default libx11-dev
```

- d. pgplot installation

```
sudo apt-get install pgplot5
```

- e. qtcreator installation

```
sudo apt-get install qtcreator
```

From this point on, the kSEMAW installation starts. To avoid troubles, user should not modify the default paths.

1. download `ksemaw-0.9.1.tar.gz` and extract the contained folder `Workspace` in the own home folder, for example `/home/user`
2. open a terminal and move to the directory
`/home/user/Workspace/qtSource/ksemaw`
by typing the command

```
cd /home/user/Workspace/qtSource/ksemaw
```

3. check the executability of the two files `semaw.shcf` and `ksemawf_startup`; if not possible, type the commands

```
chmod +x semaw.shcf
chmod +x ksemawf_startup
```

4. compile FORTRAN sources with the command

```
./semaw.shcf
```

5. compile the project `ksemaw.pro` with the command

```
qmake
```

6. complete with the command

```
make
```

and goto item 9.

Alternatively, if one wants to study the C++ sources, launch QtCreator by the application menu (generally, similarly to Windows desktop, there is a button on the left of the bottom panel) and open the file `ksemaw.pro` in the folder `Workspace/qtSource/ksemaw`. Then agree to the request “configure project” and set all the paths to

```
“/home/user/Workspace/qtSource/ksemaw”
```

7. expand `ksemaw` in the left window, edit `ksemaw.pro` and verify the presence of the two lines

```
QT += core gui
greaterThan(QT_MAJOR_VERSION, 4): QT += widgets
```

soon after the header; otherwise please add them.

8. compile by clicking the play button (green triangle) on the bottom-left; when completed, the GUI software will pop-up.
9. create an icon desktop launcher: right-click on the desktop, create launcher, name it `ksemaw 0.9.6`, and set command as

```
/home/user/Workspace/qtSource/ksemaw/ksemaw
```

set the option “open in a terminal” in order to pop-up a terminal window at the launch of the software. Finally set the working directory as `/home/$USER/Workspace`. The icon can be set to your liking

10. launch the software by clicking on the above-created icon-launcher; if required enable “make executable”

NB: the two scripts `ksemaw_startup` and `ksemawf_startup` must be executable; when `pgplot` has been installed by source, de-comment the first two rows.

NB2: because `kSEMAW` software is continuously developing, for security reasons, please make a copy of the old source folder, for example by renaming it by adding the version number.

At the first launch, the user should load one of the `.Spj` project files provided with the distribution zip-file, in order to verify that the software good working; as an example by selecting `ito_/_ve001.1.Spj` several fields in the “Valin” TAB will be automatically filled; surfing to the “Model” TAB, one will observe that the optical model consists of two layer, an inhomogeneous film 2515 Å thick on a 1 mm thick substrate. Surfing to “simulation”

TAB and click the button “Plot Exp. Measures!” four windows λ - Tn , λ - Rn , λ - n and λ - k will pop-up: the first two show the transmittance and reflectance spectra; the other two the plots of n_λ e k_λ solutions stored in the file `iito_ve001.3.nk`.

2.2 Virtual machine importation where kSEMAW is pre-installed

The importation of a virtual machine where kSEMAW is pre-installed is certainly the easiest method suitable for every OS (Linux, Windows, Mac 32/64bit) for which the virtualisation software VirtualBox is available and freely downloadable from

<https://www.virtualbox.org/>.

Once installed, the following step is to import the pre-configured virtual machine in VirtualBox. Launch the virtual machine (user=user and password=user) by clicking on the desktop icon *ksema*.

This installation option has the great advantage of NOT affecting the host OS; it requires ≈ 7 GB and it offers a ready-to-use Linux machine, reach of a quite complete software suite.

File transfer from and to the virtual machine can be accomplished by network or by a shared folder.

2.3 Installation on a virtual machine

Another interesting possibility is to install a virtual machine from scratch; to do that the steps are:

1. check if the virtualisation option is enabled in the host machine BIOS; in such a way the virtual machine is allowed to directly access the CPU, without passing through the host OS.
2. download and install the latest version of Oracle VirtualBox together with its Extension Pack from <https://www.virtualbox.org/wiki/Downloads>.
3. choose a Linux distro, for example Linux Mint (Debian based) or Linux Manjaro (Arch Linux based); concerning the Desktop Environment, XFCE is one of the lighter ones. In the case of limited amount of volatile memory (less than 4 GB) please use the 32 bit version, otherwise 64 bit is recommended.
4. set the virtual machine as: volatile memory not less than 2048 MB, graphical memory 128 Mb, HD 20 GB, enable I/O apic, some of the available processors, enable VT-X acceleration, set one folder of the host PC as shared, enable “automatic mount”.
5. launch the machine and select the ISO image of the downloaded Linux distro; follow the installation process by adopting the default options. Please note that the virtual machine installation has not effect on the host OS, but only on the virtual one. Set username and password, for example “user” and “user”. After the OS installation completion, install vbox guest addition, which is also needed for scaling the screen resolution. In the virtualbox menu, click on Devices→“insert the cd guest addition image” and then execute the Linux package: `VBoxLinuxAddition.run`; to that purpose, open a terminal, change directory to VirtualBox Guest Additions folder by typing `cd /media/user/VBox_GAs_6.0.8/` followed by

`sudo ./VBoxLinuxAdditions.run,`
giving the password (in the example, “user”); when the process is terminated, please re-boot.

6. set the privilege to use the shared folder: launch the Linux application user manager from the menu and add “user” to the vboxsf group.
7. install kSEMAW by following the instructions reported in Section 2.1.

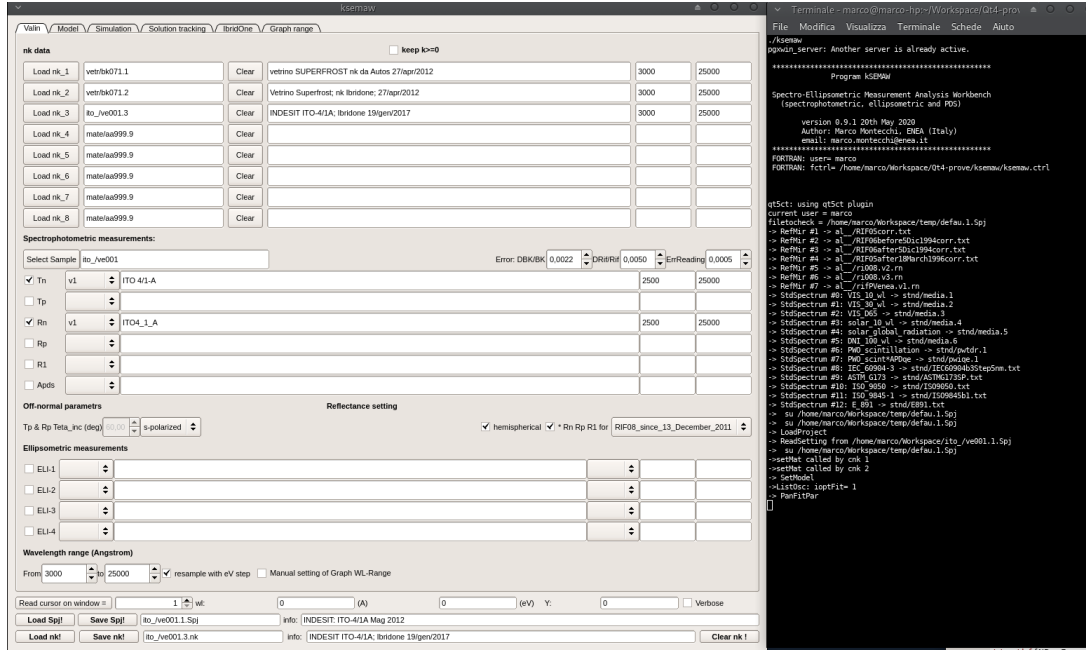


Figure 2: Graphical interface and terminal of kSEMAW.

3 How to use kSEMAW

Two windows pop-up when kSEMAW starts: the GUI and a Linux terminal; the latter shows the progress of the workflow in the two C++ (**ksemaw**) and FORTRAN (**ksemawf**) executables; messages from C++ are preceded by “->”.

The GUI is composed by a top part, structured in 6 “tabs”, ordered in logical sequence, and a bottom part, which is always visible.

The 6 TABs are:

1. **Valin**: selection of nk -files and measurements to be imported in the analysis work bench.
2. **Model**: setting of the optical device model.
3. **Simulation**: simulation of measurements on the basis of known (n, k) . When an oscillators model is set to model the unknown layer its $n(\lambda)$ and $k(\lambda)$ are also plotted.
4. **Solution tracking**: (n_λ, k_λ) solution search in tracking mode in the spaces (λ, n) and (λ, k) .
5. **IbridOne**: iterative procedure:

step-1: $n(\lambda)$ model

step-2: $k(\lambda)$ computing from $T(\lambda)$ given $n(\lambda)$

step-3: best-fit of $R(\lambda)$ with $n = n(\lambda, p_1, p_2, \dots, p_M)$ by close loop on these 3 steps.

6. **Graph range**: management of XY plots.

The bottom part, always visible, contains

- reading the cursor position on one of the opened windows
- loading/saving the SEMAW project file (`.Spj`)
- loading/saving the file with the solutions n_λ, k_λ (`.nk`).

Concerning the latter point, even if the concept could be not perfectly clear at the first reading, one has to fully understand the deep difference between n_λ, k_λ data loaded as that solution file, and the other file- nk settable in the upper part of Valin TAB: only the latter can be used in the optical model; the solution file n_λ, k_λ is the way to save the new computed values to the hard disk or to reload in the current session some previously computed or known values; these values will be shown in the λ - n e λ - k plots just for comparison purpose. Therefore, in order to use the computed solutions n_λ, k_λ in the model, the user has to save them in a file, and then add that file to the other file- nk already selected in the Valin TAB.

NB: generally speaking, commands in the GUI are written in bold and followed by an exclamation mark.

NB: before surfing to another TAB from Valin, user must name and save the current project `.Spj`!

NB: some field/functions are enabled/disabled according to their relevance in the chosen configuration.

Another important point the user should understand is the adopted philosophy for naming files and folders: kSEMAW is a software to perform the optical characterization of specimens on the basis of experimental measurements. With time the user will have to manage a multitude of files: some will concern experimental measurements, maybe achieved at different times/conditions; others will represent simulated measurements; others more will be files containing n_λ, k_λ data; finally there is the project file, which is the supporting column of the software.

All those files are in the directory `/home/$USER/Workspace`, organized in specific subdirectories for each given material/device. The single specimen has to be uniquely identified by a **nameBase**; all the files related to it must begin by **nameBase** adding suitable extensions shown in Table I, where $N = 0, 1, 2, \dots, 9$; $t = \text{“v”}$ if in UV-VIS-NIR range, otherwise $t = \text{“i”}$ for IR range.

Please note that the “near normal incidence” condition applies when the incidence angle is not greater than 10° : as a matter of fact in that angular range measurements do not depend from incidence angle or light-polarization, i.e. the difference is lower than the experimental measurement error.

Finally we remark that there is no specific limit on the number of characters for naming folders and specimens but the whole path (for example

`/home/marco/Workspace/ito_/ve001.v1.tn`) must not be longer than 256 characters. Moreover, please note that the filename cannot include blank characters.

A short description of each TAB is contained in the following paragraphs.

| File typology | nameBase extensions |
|---------------------------------------|---------------------|
| Project | .N.Spj |
| Transmittance at normal incidence | .tN.tn |
| Transmittance with polarized light | .tN.tp |
| Reflectance at normal incidence | .tN.rn |
| Reflectance with polarized light | .tN.rp |
| Reflectance measured on the back side | .tN.r1 |
| PDS absorptance | .tN.an |
| Ellipsometric measurement | .N.el |
| $n-k$ | .N.nk |

Table I: Extensions of `nameBase`.

3.1 Valin TAB

When kSEMAW starts, by default the GUI shows the Valin TAB; here file- nk and experimental measurements can be set (see Fig. 3).

The block “**nk data**” allows one to set up to 8 file- nk . Some of them could be not strictly related to the specimen under investigation; as an example, one file could contain the complex refractive index of the substrate, another the data reported in literature for the given material, and so on.

When the checkbox “keep $k \geq 0$ ” is checked, the file- nk data are resampled by forcing to 0 any negative k value.

The file- nk must be arranged according to the following format:

```
INDESIT IT0-4/1A Ibridone 2/mag/2012
201
3000.0000  1.7586253  0.16867028      2.32177973E-03  9.28342342E-04
3013.2583  1.7548164  0.16510771      2.28923559E-03  7.98091292E-04

24115.756  1.3432308  5.45175299E-02  2.32040882E-03  6.11269847E-04
25000.000  1.3170766  6.40117005E-02  2.61688232E-03  6.28869981E-04
```

More precisely, the first row is dedicated to a short info about the file (maximum 76 characters); the second one contains the number of the following records, each one composed by the values $\lambda(\text{\AA})$, n , k , $ERRn$, $ERRk$, separated by one space or tab; here $ERRn$ and $ERRk$ are the absolute errors on n and k , respectively. Data must be ordered with decreasing/increasing wavelength; the wavelength step is not required to be constant.

NB: Angstrom (\AA) is the adopted unit for wavelength and *thin* film thickness (millimetre for the *thick* ones); conversely the nanometre (nm) is used in the experimental files SF, ELI e PDS!

Each file- nk has a row in the GUI where the first field on the right of `name_file` shows the file info; the following other two fields show λ_{min} and λ_{max} of the data wavelength range; these fields are just informative and cannot be edited.

The experimental measurements can be set in the block “**Spectrophotometric measurements**”. A dialog window for file selection will pop-up when “Select Sample” is pressed; it is sufficient to select just one of the files concerning the specimen of interest

ksemaw

Valin / Model / Simulation / Solution tracking / IbridOne / Graph range

nk data ☐ keep k>=0

| | | | | | |
|-----------|--------------|-------|--|------|-------|
| Load nk_1 | vetr/bk071.1 | Clear | vetrino SUPERFROST nk da Autos 27/apr/2012 | 3000 | 25000 |
| Load nk_2 | vetr/bk071.2 | Clear | Vetrino Superfrost; nk Ibridone; 27/apr/2012 | 3000 | 25000 |
| Load nk_3 | ito_ve001.3 | Clear | INDESIT ITO-4/1A; Ibridone 19/gen/2017 | 3000 | 25000 |
| Load nk_4 | mate/aa999.9 | Clear | | | |
| Load nk_5 | mate/aa999.9 | Clear | | | |
| Load nk_6 | mate/aa999.9 | Clear | | | |
| Load nk_7 | mate/aa999.9 | Clear | | | |
| Load nk_8 | mate/aa999.9 | Clear | | | |

Spectrophotometric measurements:

Select Sample: ito_ve001 Error: DBK/BK 0,0022 Drift/Rf 0,0050 ErrReading 0,0005

| | | | | |
|--|----|-----------|------|-------|
| <input checked="" type="checkbox"/> Tn | v1 | ITO 4/1-A | 2500 | 25000 |
| <input type="checkbox"/> Tp | | | | |
| <input checked="" type="checkbox"/> Rn | v1 | ITO4_1_A | 2500 | 25000 |
| <input type="checkbox"/> Rp | | | | |
| <input type="checkbox"/> R1 | | | | |
| <input type="checkbox"/> Apds | | | | |

Off-normal parameters **Reflectance setting**

Tp & Rp Teta_inc (deg) 60,00 s-polarized ☒ hemispherical ☒ * Rn Rp R1 for RIF08_since_13_December_2011

Ellipsometric measurements

| | | | | |
|--------------------------------|--|--|--|--|
| <input type="checkbox"/> ELI-1 | | | | |
| <input type="checkbox"/> ELI-2 | | | | |
| <input type="checkbox"/> ELI-3 | | | | |
| <input type="checkbox"/> ELI-4 | | | | |

Wavelength range (Angstrom)

From 3000 to 25000 ☒ resample with eV step ☐ Manual setting of Graph WL-Range

Read cursor on window = 1 wf: 0 (A) 0 (eV) Y: 0 ☐ Verbose

Load Spj! Save Spj! ito_ve001.1.Spj info: INDESIT: ITO-4/1A Mag 2012

Load nk! Save nk! ito_ve001.3.nk info: INDESIT ITO-4/1A; Ibridone 19/gen/2017 Clear nk !

Figure 3: “Valin” TAB.

| | |
|-------------------------------|--|
| Riga di commento | SUB ZNSE ELICAM 5 mm 19.3.92 |
| M N | 2 72 |
| θ_1 N1 λ_min λ_max | 75.00 36 500.0 850.0 |
| θ_2 N2 λ_min λ_max | 60.00 36 500.0 850.0 |
| ... | 75.00 500.0 17.583 10.387 0.136 0.060 |
| θ_M NM λ_min λ_max | 60.00 500.0 168.283 15.016 0.150 0.036 |
| θ_1 λ_1 Δ_1 ψ_1 errΔ_1 errψ_1 | 75.00 510.0 15.948 10.584 0.129 0.060 |
| θ_1 λ_2 Δ_2 ψ_2 errΔ_2 errψ_2 | 60.00 510.0 168.840 14.686 0.142 0.035 |
| ... | ... |
| θ_M λ_N Δ_N ψ_N errΔ_N errψ_N | ... |

Figure 4: Format for ellipsometric data files; on the left (right) the structure (an example).

marked by **nameBase**, and automatically the software will locate all the available SF, ELI and PDS measurements and, in the case of multiple choice, all the options will be offered in the menu.

NB: in the case of more measurements of the same type, the files must be numbered starting from 0 and increased by 1!

Concerning the format of the SF files, all those generated by Perkin-Elmer UV-VIS-NIR and IR instruments, since 1988, are accepted.

Otherwise data should be arranged like in the following example:

```
KN929aCW_csl 10000A Tdiretta
#####SCALED%
2500.
250.
1126
2500 78.090897
2498 80.310163
.....
252 0.003400
250 0.000785
```

where the measured values are in %. In the case of absolute value, i.e. 0.78090897 instead of 78.090897, the second row has to be modified in

```
#####SCALED A
```

In any case the meaning of the first rows is:

1. info
2. value type (% or Absolute)
3. initial λ
4. final λ
5. number of data (N).

N rows consisting of the couple of values λ **val-measured** follow in decreasing/increasing order of λ ; once again the λ step can be not constant.

The format for ellipsometric data is shown in Fig. 4:

1. info
2. number of different measurements (M), total number of experimental data (N)
3. M rows, each one composed by θ , N_{data} λ_{\min} , λ_{\max}
4. N rows containing ellipsometric data are following.

Once again, the wavelength unit is nanometre. Up-to 4 ellipsometric files can be set.

NB: to be loaded into the program, the measurement of interest must be enabled by ticking the proper box.

The Valin TAB offers the possibility to set the parameters used for computing the error propagation (under the hypothesis of maximum correlation) of transmittance

$$\begin{aligned}
 T &= \frac{M}{B} \\
 \Delta T &= T \left(\frac{\Delta M}{M} + \frac{\Delta B}{B} \right) \\
 B &= 1 \rightarrow M = T \\
 \Rightarrow \Delta T &= T \Delta B + \Delta M
 \end{aligned}$$

and reflectance

$$\begin{aligned}
 R &= \frac{M}{B} R_{\text{ref}} \\
 \Delta R &= R \left(\frac{\Delta M}{M} + \frac{\Delta B}{B} + \frac{\Delta R_{\text{ref}}}{R_{\text{ref}}} \right) \\
 B &= 1 \text{ if } R_{\text{ref}} \approx 1 \\
 &\rightarrow M \approx R \\
 \Rightarrow \Delta R &= R (\Delta B + \Delta R_{\text{ref}}) + \Delta M
 \end{aligned}$$

where M is the measurement, B is the baseline, ΔB is the baseline error, ΔR_{ref} the reflectance relative error of the reference mirror, ΔM the reading error of the spectrophotometer; by default the three fields “Error: DBK/BK”, “Drif/Rif” and “ErrReading” are set to the typical values: 0.002, 0.005 e 0.0005. As will be discussed later, the measurement errors are used in kSEMAW for evaluating the uncertainty area of the solution n_λ, k_λ and then the errors on n and k .

Moreover the software offers the possibility to multiply the experimental reflectance spectra for the reference mirror reflectance, as soon as the file is loaded and re-sampled. To that purpose the user must tick the “* Rn Rp Rl for” checkbox and then select the reference mirror in the drop down menu (enabled just after the above ticking).

The drop down menu with the list of the available reference mirrors can be customized by editing the file **referenceMirrors.txt**, located in the folder **ksema**; the file is composed as follows:

```

RIF05
al__/_RIF05corr.txt
RIF06_before_5_December_1994
al__/_RIF06before5Dic1994corr.txt
RIF06_after_5_Decembre_1994
al__/_RIF06after5Dic1994corr.txt
RIF05_after_18_March_1996
al__/_RIF05after18March1996corr.txt
RIF08_since_13_December_2011
al__/_ri008.v2.rn
RIF08_after_17_January_2018
al__/_ri008.v3.rn
RIF_PV_ENEA
al__/_rifPVenea.v1.rn

```

Each reference mirror is described by a couple of rows: the first is the name to add in the menu, the second is the path, including the filename, in **Workspace**. In such a way the user can easily suppress undesired items and add those of his interest.

In the case of roughness, kSEMAW adopts the simplified approach proposed by [2] for evaluating hemispherical³ or specular (direct) reflectance (transmittance), depending on the checkbox “hemispherical” (checked or not). Please note that the choice simultaneously holds for transmittance and reflectance.

If some measurements obtained at oblique incidence is selected, the user must set the incidence angle and the polarization type (*s-polarized* or *p-polarized*); the not polarized case is not considered here because it is not useful for optical characterization purposes. Later, the incidence angle can be modified in the Simulation TAB.

As soon as file-*nk* and measurements are set, kSEMAW computes the maximum common wavelength range where data from all the selected inputs are available; the limit values of that range are shown in the field “Wavelength Range (Angstrom)”. By default, that is the range used for re-sampling both file-*nk* and experimental measurements on a common base of 201 points⁴, with step in wavelength (Å) or in energy (eV) when the checkbox “resample with eV step” is checked. The latter choice is recommended for thin film coatings because it allows to view the interference fringes with an almost regular period. Higher resolution along a narrower region can be obtained by properly adjusting the two spin boxes on the right of “eV step from”.

By default the range of the abscissa λ in the drawn plots is set to the maximum common wavelength range; otherwise by ticking “Manual setting of Graph WL-Range” the user can set a different range, both narrower or wider, by setting the limits in the first row of the “Graph range” TAB.

NB: before surfing from Valin to another TAB, the user must name and save the current project .Spj!

³reflectance/transmittance obtained by placing the specimen on the suitable port of an integrating sphere is called *hemispherical*; the purpose of that arrangement is to collect the whole radiation transmitted/reflected in the half-space.

⁴That value was set in the early days of software development in '90, on a workstation HP 9000 equipped with a 100 px wide terminal! Later we continued to keep that value because it does not slow down the solution computing in the selected wavelength range, but ensures a sufficient sampling-density to represent spectra with many interference fringes, provided the step is set to energy.

The recommended choice is “`nameBase.1.Spj`”; please note that the software automatically checks for the presence of the extension “`.Spj`”, and adds it if necessary. It can be useful to keep trace of the progress of the characterization by saving milestone projects with names differing in a numerical field only (`2.Spj`, `3.Spj`, ...).

Figure 5: “Model” TAB.

3.2 Model TAB

The Model TAB (Fig. 5) allows one to set the structure of the optical device.

The first step is setting the layer number (up-to 9) to make an equivalent number of rows, one for each layer, editable.

The first layer on the top corresponds to the one interfaced to air, i.e. the *front* side of the specimen; the bottom interface of the bottom layer is the specimen *back* side. Please note that to attribute *front* and *back* to the two sides of an optical multilayer device is quite arbitrary, except for the case of a thin film deposited on a thick substrate, where *front* normally refers to the coated side of the substrate. Anyway, once it has been established, kSEMAW considers the two reflectances with extension “rn” and “rp” as obtained with the incident radiation impinging on the *front* side of the specimen: the former at near normal incidence, the latter at oblique incidence in which case the light is polarized. Conversely the reflectance loaded with extension “r1” is assumed to be measured with the radiation impinging on the *back* side, at near normal incidence.

When the absorptance

$$A = 1 - T - R$$

is lower than the experimental error, then “rn” (front) and “r1” (back) reflectances are the same within the experimental error. Otherwise these two measurements are independent and their knowledge is very useful for optimizing the optical model.

Moreover, ellipsometric measurements are intended to be carried out on the *front* side and they have to be not affected by any contribution coming from the *back* side, which usually has to be abraded.

For each layer, the user must set *type*, *thickness* and *roughness*.

In the case of “bulk” layer, e.m. wave propagation is treated by neglecting interference among the several contributes coming by the two interfaces; layer thickness is in millimetre units.

In the case of “homo.film”, the thickness is expressed in Angstrom units, and it is assumed to be thin, so that the wave propagates in a coherent way; interference phenomena will arise by summing up the contributes coming from the two interfaces.

The same also occurs in the case of “inhomo.film”, but in this case the user can set a parabolic profile for the refractive index across the layer thickness for both n and k by means of two parameters (the film thickness is normalized to 1; it is 0 on the back and 1 on the front):

$$\begin{aligned}\frac{\Delta n}{\langle n \rangle} &= \frac{n(1) - n(0)}{\int_0^1 n(x) dx} \\ \frac{\langle n \rangle - n(0.5)}{\langle n \rangle} &= \frac{\int_0^1 n(x) dx - n(0.5)}{\int_0^1 n(x) dx}\end{aligned}$$

related to gradient and curvature of the profile, respectively. These parameters are respectively labelled as “GRAD- n ” and “CURV- n ” in the TAB; for the sake of simplicity the normalization to $\langle n \rangle$ is here omitted. Similar formulas hold for the imaginary part.

As a further possibility, by means of the input parameter “GRAD- n -slope” (eV^{-1}) the user can set “GRAD- n ” as linearly changing with the photon energy, thus

$$\frac{\Delta n}{\langle n \rangle}(E) = \frac{\Delta n}{\langle n \rangle}(0) + qE$$

where q is the value set as “GRAD- n -slope” and $\frac{\Delta n}{\langle n \rangle}(0)$ is the one set in “GRAD- n ”. We benefited of this further option for characterizing LiF film with many fringes in the UV-VIS-NIR range.

The computation is performed by subdividing the inhomogeneous layer in a number of homogeneous sub-films with refractive index suitably set for modelling the profile; 23 is their default number.

NB: n, k of the inhomogeneous layer refer to the mean value $\langle n \rangle$ and $\langle k \rangle$ as computed along the thickness.

The effect of roughness is evaluated according to the method described in [2]. More precisely, hemispherical and specular reflectance are respectively evaluated as the statistic average on the roughness ($\langle \cdot \rangle_\delta$) after and before computing the square of the reflectance complex coefficients, that is

$$\begin{aligned}R_{\text{hemispherical}} &= \langle |r(x, y)|^2 \rangle_\delta \\ R_{\text{specular}} &= |\langle r(x, y) \rangle_\delta|^2.\end{aligned}$$

Roughness can be considered as a variation of the film/substrate thickness; its effect is here numerically computed as the mean value on $2N + 1$ different thickness values, distributed around the Gaussian peak, in the range $[-3\sigma, 3\sigma]$. The number of discretization can be set in “computing $\langle x \rangle$ with N ” ($N = 3$ by default; $2 \leq N \leq 5$).

Once the layer type is set (bulk, homo or inhom), the user has to assign at each layer a material chosen among those listed in Materials (Material #j) in the lower part of the TAB; each material can be set in 5 different ways, by the drop down menu on the left:

1. nk constant;
2. nk by fit option “Fit #M” with $1 \leq M \leq 7$;
3. nk from one of the file- nk , previously loaded in Valin TAB;
4. nk computed in the current session with IbridOne;
5. nk unknown.

Please note that Material #1 is reserved to nk unknown by default. Only when kSEMAW is used to simulate measurements, the user must assign nk unknown to one of the known (n, k) by surfing to Simulation TAB and selecting in the field “nk-unknown” one of the above described options (as an example, the name of one of the file- nk already set in Valin).

As a further option, by ticking the box in the “with” column, the user can set a second material in such a way that n, k of Material #j are computed according to the Equivalent Medium Approximation, that is as a mixture of the two materials (the first on the left, the second on the right) with the ratio f , displayed in the last field of the row.

Finally, by ticking the box “Symmetric on second face” the user can set a specular multilayer on the back side of the lower layer. As an example, if the device consists of a thin film on a substrate, this option adds a specular film on the back side of the substrate; if the front film has a growing index profile towards the substrate, the same will hold for the film added to the rear side. That option can be used for substrates treated with sol-gel dipping coating.

NB: once a multilayer is set, the layer order can be modified by the “dw” and “up” buttons for each layer. By increasing (+1) the layer number, a new layer is added on the front side; oppositely, by decreasing it (-1), the first layer on the front side is cancelled.

The screenshot shows the 'Simulation' TAB in the ksemaw software. The top section, labeled 'nk-unknown', contains input fields for 'Fit #1' (set to 1), 'n' (1.99942), and 'k' (0.0017122). Below this is a table of 20 oscillators. The first three oscillators are checked: Osc 1 (Quant-homo, C=28.1772, E0=5.5, D=0.0400342, K=0), Osc 2 (Quant-homo, C=7.90049, E0=0.345009, D=0.0146247, K=0), and Osc 3 (Flat, C=1.48451, E0=0, D=0, K=0). The rest are unchecked. Below the table, there's a 'Theta' section with checkboxes for 'Tn', 'Tp', 'Rn', 'Rp', 'R1', 'Apds', and 'DEL-1' through 'DEL-4'. The 'Rn' checkbox is checked. To the right of these are input fields for 'D/Err RMS', '<Exp.>', and '<Sim.>'. Below this is a 'COMMANDS' section with buttons for 'Plot exp. measures!', 'Simulate!', 'Save Sim!', and 'Plot Absorptance at each layer!'. The bottom status bar shows file loading and saving options, including 'Load Spj!', 'Save Spj!', 'Load nk!', and 'Save nk!'.

Figure 6: “Simulation” TAB.

3.3 Simulation TAB

The Simulation TAB (Fig. 6) allows to compute simulated curves and to compare them with the experimental data.

As a first step the user has to set “nk-unknown” in the first row of this TAB, in a similar way to what described in the previous section.

If one of the 7 available fit options is selected, the oscillators functions composing it are those signed by a ticked checkbox among the 20 records shown below. Working on these records the user can add new oscillators, modify the current ones or set a totally new fit option. In any case please keep in mind that 20 is the maximum number of available oscillators.

NB: the same oscillator should not be shared among different fit options because there is a unique place for storing the parameter values, which depends on the oscillator sequential number and not by the fit option to which it is associated.

In the drop down menu of each oscillator, the user can choose among 9 typologies:

- Lorentz

- Quant-homo
- Quant-inhomo
- Flat
- Drude
- Direct Gap Cody
- Direct Gap Tauc
- Indirect Gap Cody
- Indirect Gap Tauc

The detailed description of these oscillators functions and their physical meaning are reported in Appendix A.

Once nk-unknown has been set, kSEMAW can compute the curves simulated according to the optical model of the devices already set in the Model TAB.

If experimental measurements are available, the user has to select the ones of interest; then by pushing “Plot exp. Measures!” a number of windows will pop-up: one for each selected experimental measurement, plus the two λ - n and λ - k with the graphs of $n(\lambda)$ and $k(\lambda)$. Two more windows with the graphs of $\epsilon_{\text{psi1}}(\lambda)$ and $\epsilon_{\text{psi2}}(\lambda)$, respectively real and imaginary part of the permittivity, will pop-up when the checkbox “Plot ϵ_{psi1} ϵ_{psi2} ” is checked.

NB: once opened, these windows can (and must) not be closed.

If the resolution of the screen was not high enough to contain all such windows, the less relevant ones can be reduce to icon, or covered by the most important windows. Analogously, the small window “PgPlot server”, can be reduced to icon, but not closed.

NB: the scale control of all the graphs is in Graph-Range TAB, described in 3.6. There the user can also resize the graphs and set the line thickness; to make the latter effective, please save the project and re-launch kSEMAW.

By pushing “Simulate!”, the simulated curves will be added to the opened graphs as dashed-lines to be distinguishable from the experimental ones, which are drawn as dot-symbols.

The bottom left form is structured as a matrix and reports for each measurements: i) RMS deviation (normalized to the error) between experimental and simulated spectrum (D/Err RMS); ii) mean value, averaged with the spectrum specified in “Average type” combobox, of the experimental spectrum ($< Exp. >$); iii) idem but for the simulated spectrum ($< Sim. >$).

The drop down menu of “Average type” can be easily customized by editing the file `standardSpectra.txt`, located in the folder `ksemaw`, by default set to:

```
VIS_10_w1
stnd/media.1
VIS_30_w1
```

```
stnd/media.2
VIS_D65
stnd/media.3
solar_10_wl
stnd/media.4
solar_global_radiation
stnd/media.5
DNI_100_wl
stnd/media.6
PWO_scintillation
stnd/pwtdr.1
PWO_scint*APDqe
stnd/pwqe.1
IEC_60904-3
stnd/IEC60904b3Step5nm.txt
ASTM_G173
stnd/ASTMG173SP.txt
ISO_9050
stnd/ISO9050.txt
ISO_9845-1
stnd/ISO9845b1.txt
E_891
stnd/E891.txt
```

where each standard spectrum is described by a couple of lines: the first one contains its name appearing in the menu, the second one the full path in the work folder **Workspace**. The user is allowed to suppress undesired voices or add new ones.

The default menu is composed by:

- VIS 10 wl
- VIS 30 wl
- VIS D65
- solar 10 wl
- solar global radiation
- DNI 100 wl
- PWO scintillation
- PWO scintillation * APDqe
- IEC 60904-3
- ASTM G173
- ISO 9050
- ISO 9845-1

- E 891

This list tracks the use (and development!) I made of the software along about 30 years, first dealing with the energy standard for architectural glazings, then the CMS experiment at LHC of CERN, and finally concentrated solar power (CSP).

Pushing the “Simulate!” button, both experimental (re-sampled on 201 points) and simulated curves are automatically saved on hard disk in the directory “**expo**” with the names

- **MisSFexp.dat** spectrophotometric experimental measurements (SF)
- **MisSFexpErr.dat** errors of the above ones
- **MisEliexp.dat** ellipsometric experimental measurements (ELI)
- **MisEliexpErr.dat** errors of the above ones
- **MisSim.dat** simulated curves

All these files are continuously overwritten with the most recent values; in order to save them permanently on hard disk, on a customized location and name, the user should push the button “Save Sim!”.

The n, k values used for the simulation will be written in “temp” from scratch if the checkbox “ $nk \rightarrow$ temp from scratch” is checked; then, by means of the last row of the GUI, the user can save those data as a file- nk on the hard disk.

When the checkbox “Sim \rightarrow Exp!” is checked, the simulated values are overwritten on the experimental ones. From that point on the user will work on *synthetic* measurements as if they were *experimental*.

By pushing the button “Plot Absorptance at each layer !” the absorptance spectra obtained right at the exit of each *thin* layer will be plotted, considering the subsequent layer as the output medium. Generally the absorptance increases layer after layer, but because of the interference some small inversion of such a trend can occur. The absorptance spectra are automatically saved in the directory “**expo**” as individual files named **Abs#j.dat**.

Finally by pushing “Plot <T>,<R>,<R1> vs theta”, the graph of mean values averaged over the selected standard spectrum of transmittance, reflectance and back-reflectance versus the incidence angle and for the selected polarization will pop-up; the polarization can be set by its drop down menu (s-polarized, p-polarized and unpolarized).

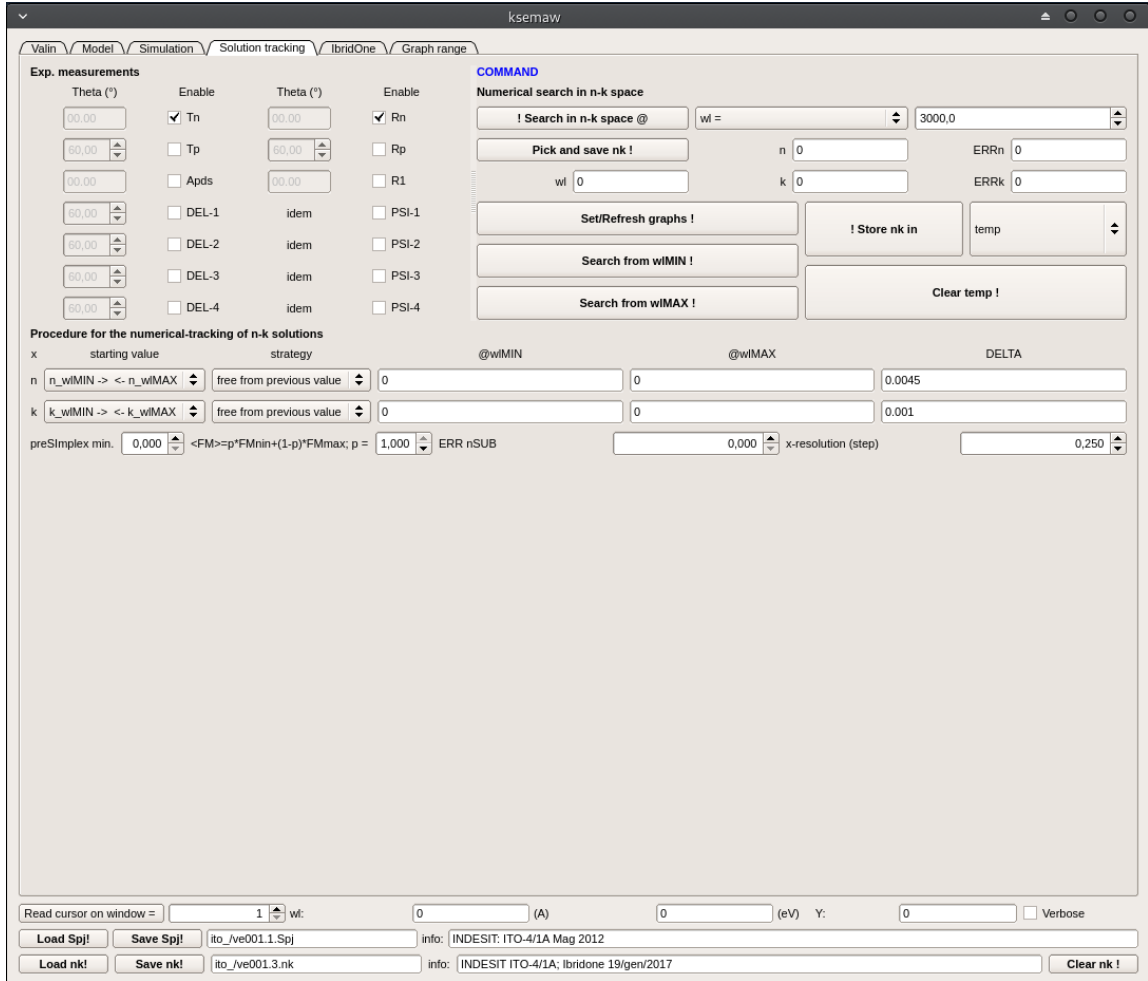


Figure 7: “Solution tracking” TAB.

3.4 TAB Solution tracking

One of the two methods offered by kSEMAW for evaluating the complex refractive index of one layer of the optical device is named “Solution Tracking”, managed by the Solution-tracking TAB (Fig. 7).

As a first step, the user has to tick the measurements, among the loaded ones, he wants to consider for the solution search.

NB: this selection must be done in this TAB even for the IbridOne method, managed by the next TAB.

The following step is to surf to the Graph_range TAB to set the n and k search-ranges. Coming back to the Solution_tracking TAB, two windows will pop-up automatically, or will be refreshed if already opened: $n(\lambda)$ and $k(\lambda)$. Please note that if a solution file n_λ, k_λ has been loaded (last row of the GUI) or some previously computed solutions have been saved in the temporary memory, they will be plotted as vertical bars which height corresponds to the error. The graphs will be refreshed by pushing “Set/refresh graphs !”.

Before starting the tracking search, the user has to set the parameters displayed in the form “Procedure for the numerical-tracking of n-k solution”. In the left drop down menu (separately for n and k) three options are available to set the initial value for $n(\lambda)$

and $k(\lambda)$ solution search:

1. constant values set in the fields @wlMIN and @wlMAX, to be used if the search starts from minimum or maximum wavelength respectively
2. computed values by Fit#M option
3. values from one of the loaded file- nk

Then the user has to set the *strategy* to adopt when moving from one lambda to the next among the following options:

- (i) free from previous value
- (ii) free from starting value
- (iii) forced to starting value

In the latter case the value is fixed to the initial one without any optimization; this option is very useful when only one measurement is available and only one of the two unknown n, k can be determined: the other is kept to the literature values.

In the case of option #1, in order to obtain reasonable values to set in the fields @wlMIN e @wlMAX, the user has to launch the command “! Search in n-k space @”, at the wavelength selected by the right drop down menu; in the case of “wl=”, the value set in the field on the right is used. At that command, if not already opened, a window with the plot of the chosen (n, k) range will pop-up; that graph will show, for each measurement, a belt containing the (n_λ, k_λ) points which allow to reproduce the experimental value within the error; if the error is null, the belt will collapse to a single line. The intersection area between the (n_λ, k_λ) belts obtained from different measurements represents the common solution area.

Generally speaking, at each wavelength, zero, one or more solutions (i.e. couples of n_λ, k_λ values) can exist, because of the transcendent nature of the equations describing the optical features of the multilayer. Among all these mathematical solutions, only one has a physical meaning; the user should identify it and insert its n_λ, k_λ values below “wlMIN” or “wlMAX”, according to the wavelength. Please note that the following fields, in the “DELTA” column, display the last numerical step used along the solution tracking of n and k ; these values are automatically set during the computation and generally no intervention by the user is required.

Once suitable initial (n_λ, k_λ) values have been set, the user can launch the solution tracking search, where the wavelength is modified step by step, starting from the initial one until the limit of the range. During that process, the user should read the messages displayed in the terminal. As an example, in the case of the *free from previous value* strategy, the search stops when n goes out of the search range; by left clicking on a point of the n graph, the selected value is used for restarting the search; otherwise the user can terminate the search by right clicking, returning the flow control to the GUI (the message “scrivo done!” will be printed in the terminal). Until one of these two instructions is given, the GUI remains locked. Please note that the solution tracking search can be launched from both “wlMIN” or “wlMAX”.

Undoubtedly the simplest case is the search of solutions (n_λ, k_λ) for a bare substrate: if the (n, k) search range is suitably sized, the obtained solution will cover the whole

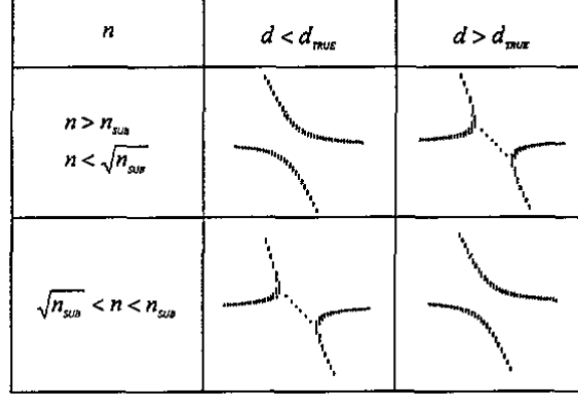


Figure 8: Discontinuity typology affecting the solution crossings related to odd extremes, in the λ - n space, caused by a wrong thickness value.

wavelength range and appear well connected. The substrate thickness can not be optimised on the basis of the optical measurements, and it must be measured by a calipers or a thickness gauge. A possible problem is an anomalous behaviour of n_λ caused by some measurement imperfection or, more rarely, due to the substrate roughness. Before increasing the model complexity, the user should experimentally verify the presence of roughness, for example by measuring the amount of scattered radiation. Finally, in the case of float glasses, the UV reflectance measured on one side could differ from the one measured on the other side, because the refractive index is a bit different between the two sides of the substrate.

The case of thin films is more difficult: the solutions in the (λ, n) space are arranged to form branches which draw a sort of *solution crossings*; as a general rule, such crossings are situated in correspondence of even and near odd interference fringe extremes. A simple way to discriminate between even and odd extremes is by drawing the transmittance/reflectance of the bare substrate (in Simulation TAB set nk-unknown=nk-substrato) and overlapping the reflectance/transmittance graph to that of λ - n : even extremes of reflectance/transmittance fringes are those closer to the bare substrate curve.

At the beginning the model is not optimized and the solution crossings will appear not well connected. The discontinuities can be suppressed or at least reduced by adjusting the model parameters (thickness, roughness, gradient, ecc.). Fortunately, as will be illustrated, the parameters can be optimized according to precise criteria.

The film thickness is the first parameter one should optimize; for low absorption it can be shown [5] that a wrong thickness value can give rise, at the odd crossings, to discontinuities of different types as explained in Fig. 8.

A similar analysis has been performed on thin films with refractive index having a parabolic profile along the thickness [3, 4]; full details are given in the indicated papers, here we just recall some information for the most common case of inhomogeneity for the real part n .

The gradient of n mainly affects the even crossings. If that is the case, the user should surf to Model TAB, set “inhomo film” (if the actual setting was “homo film”) and adjust the value of n gradient on the basis of Fig. 9.

The presence of n curvature is revealed by the impossibility to connect all the odd crossings using the same thickness value. If the examined wavelength range contains both $m = 1$ and $m = 3$ crossings, then the true thickness value is between d_1 and d_3 . The user

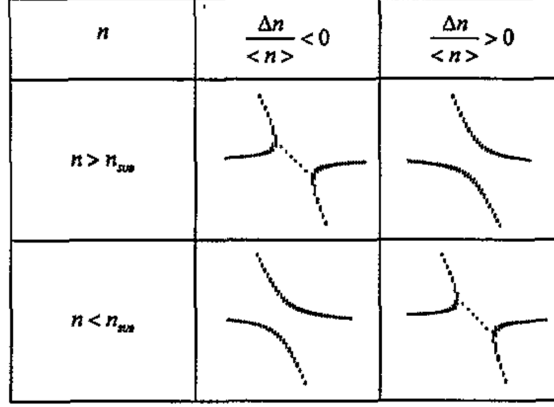


Figure 9: Discontinuity affecting even crossings due to n gradient.

should adjust the curvature value to achieve the simultaneous connection of $m = 1$ and $m = 3$ crossing for the same thickness. Please note that d_m , i.e. the thickness optimized at m crossing, decreases (increases) for positive (negative) curvature.

Once the solution crossings are well connected, the identification of the solution sub-ensemble having a physical meaning is quite easy. From this point on the user has two options:

1. to save them in a file- nk to be loaded in the TAB “Valin”; the nk -values will be resampled by the internal subroutine of kSEMAW and will be available for the model setting;
2. to arrange a suitable composition of oscillators in the Tab “Simulation” for best fitting the n -values by mean of the specific tools available in the Tab “IbridOne” described in the next section.

In any case, the computed nk -values can be saved by pushing the button “!Store nk in” to store the values in the vector “temp” (by default) or in one of the 8 file- nk ($N=1, 2, \dots, 8$) as offered by the drop down menu on the right. In the latter case please note that the saving is valid only if one solution is present at each sampled wavelength; otherwise the recommended way is the solution saving in “temp” and then in a file which will be loaded in the TAB “Valin”. More precisely, the values stored in “temp” can be permanently saved on the hard disk by pushing the “Save nk!” button in the last row of the GUI; if the field on the right is already filled with a valid path, then that old file will be overwritten with the fresher values stored in “temp” (a warning message will pop-up), otherwise the user will be asked to set the path to a new file by a dialog window. As usual the use of **nomeBase** followed by a numerical character is strongly recommended; in such a way one can save up-to 10 different file- nk concerning to the same specimen. Moreover the user should also fill the field “info” to store information about the file.

Please note that each time new solutions are temporary saved in “temp”, they are added to the ones already stored there; to erase the previously saved values, the user should push the “Clear temp!” button.

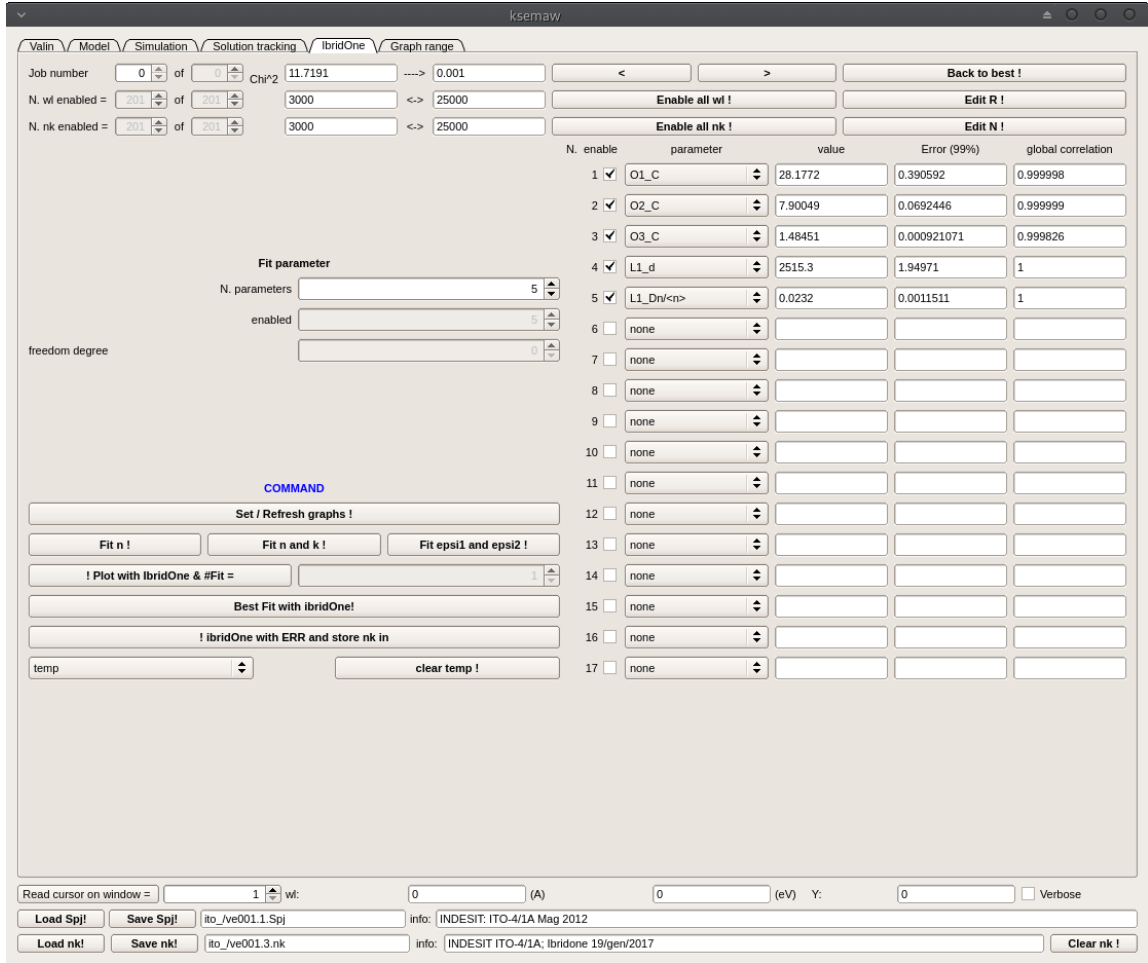


Figure 10: “IbridOne” TAB.

3.5 IbridOne TAB

The IbridOne TAB (Fig. 10) allows one to manage the homonymous method for evaluating n - k solutions.

The name *IbridOne* is the synthesis of the words *Ibrido* (i.e. hybrid in Italian) and number *One*, referring to a first version of an innovative hybrid computing method where the $n(\lambda)$ behaviour is modelled by a set of suitable analytical functions (Lorentz, Drude, ecc.) depending on a number of parameters to be optimized; the initial value of these parameters must be good enough to give a first reasonable evaluation of $n(\lambda)$. Once the $n(\lambda)$ behaviour is set, $k(\lambda)$ is evaluated so to perfectly reproduce the experimental $T(\lambda)$ spectrum. Once $n(\lambda)$ and $k(\lambda)$ are known, the software computes the simulated $R_{cal}(\lambda)$ spectrum, and compares it with the experimental $R_{exp}(\lambda)$ one by means of a merit function $\chi^2 = \sum_i (R_{cal}(\lambda_i) - R_{exp}(\lambda_i))^2 / \Delta R_i^2$ calculated over the whole set of λ_i used for resampling. This merit function is passed to the Levenberg-Marquardt non-linear least square routine (part of the MINPACK library) for optimize the parameters of the optical model (thickness, gradient, curvature, ...) as well as the enabled parameters of the functions used to describe $n(\lambda)$. Please note that by definition the transmittance spectrum is always perfectly reproduced.

NB: *IbridOne* can be used only after a suitable Fit#j option has been set in

the Simulation TAB (see section 3.3). Moreover in the Solution-tracking TAB the user must tick a couple of measurements: one transmittance (mandatory) and at least one reflectance / Ψ .

NB: in order to choose the most proper functions for modelling $n(\lambda)$ in *IbridOne*, the user should initially use the solution-tracking mode to select a reasonable solution set; then he has to arrange a suitable fit option for modelling $n(\lambda)$.

Another preliminary operation is to verify the suitability of the n and k ranges (set in Graph-range TAB) where solutions will be searched. Then, by surfing to the IbridOne TAB, three windows containing the plots of $n(\lambda)$, $k(\lambda)$ and $R(\lambda)$ or $\Psi(\lambda)$ (according to the one selected in the TAB Solution-tracking) will pop-up or will be refreshed. In any case by pushing the “Set/Refresh graphs !” button, these windows will be refreshed. If the checkbox “Plot epsi1 epsi2” has been checked in the Simulation TAB, other two windows with the plots of $\epsilon_1(\lambda)$ and $\epsilon_2(\lambda)$ will be shown/refreshed. Once again, please verify the ranges for ϵ_1 and ϵ_2 in the Graph-range TAB.

By pushing the “plot with ibridOne & #Fit= !” button, a single computing run of IbridOne is launched, with the fit option already set, on the basis of the current parameter values, without optimization; the results are shown as new $n(\lambda)$, $k(\lambda)$ and $R(\lambda)$ curves in the opened windows. Moreover each graph will include the (n_λ, k_λ) solutions already computed/loaded and the experimental $R_{exp}(\lambda)$.

The “Best Fit with ibridOne!” button launches the IbridOne procedure together with the best fitting of the parameters listed in the “parameter” column and enabled by checking the “enable” checkbox. The user can set the displayed parameters by the individual drop-down menu, while their total number is set by the spin box “N. parameter”

NB: IbridOne can be launched only if at least one parameter has been enabled for the best-fitting.

Once satisfactory results are obtained, by pushing the “! ibridOne with ERR and store nk in ” button, nk values and their error (based on the experimental errors) are computed, provided that at least one parameter is left free to be optimized; otherwise errors are not evaluated. Similarly to what already described for the solution-tracking, nk data are only temporarily saved (i.e. in the current software session) in the location set in the drop-down menu at the row below. The permanent saving is achieved by pushing “Save nk!” at the GUI bottom, where of course filename and info string can be modified at any time.

Please note that each time new solutions are temporarily saved in “temp”, they are added to the ones already stored there; to erase the previously saved values, the user should push the “Clear temp!” button.

In the second row of the TAB, the button “EditR!” allows the user to disable some reflectance data from the best-fit; please follow the instructions that will be displayed in the terminal.

As mentioned in the previous section, the parameters of the built up fit option can be best-fitted over the data of n only by pushing “Fit n!” at the IbridOne TAB; those data can be the ones computed by ksemaw or uploaded by the file- nk (last row of the GUI). Before launching the best fit procedure, all the parameters concerning the device

optical model will be automatically disabled. In the 3rd row of this TAB, the commands for excluding part of n data are available; the user has to follow the instructions that will be displayed in the terminal. If also k values are important to optimize the chosen oscillator, the user should push the “Fit n and k!” button; in such a way the best fit runs over both n and k data. As a further option, the best fit can be performed over ϵ_1 and ϵ_2 data when the “Fit epsi1 and epsi2 !” button is pushed.

The two buttons “<” and “>” on the top-right allow to browse the results obtained during all IbridOne runs in the current session. The user can also set the parameters back to the values got in the run with with the lowest χ^2 by pushing “Back to best!”.

The screenshot shows the 'Graph range' TAB in the ksemaw software. The interface is divided into two main sections: 'ABSCISSA' and 'ORDINATE'. The 'ABSCISSA' section has a 'set eV scale' checkbox and four columns: Xmin, Xmax, VALmin, and VALmax. The 'ORDINATE' section has four columns: Ymin, Ymax, VALmin, and VALmax. The 'graph' row at the bottom has three editable fields: 6, 0.5, and 3. The status bar at the bottom shows file names and a 'Clear nk!' button.

| ABSCISSA | | set eV scale | | | | units |
|----------------|------|--------------|------------|----------|------------------------------------|-------|
| | Xmin | Xmax | VALmin | VALmax | | |
| X | 3000 | 25000 | 3000 | 25000 | Angstrom | |
| d | 0 | 0 | 0 | 0 | Angstrom | |
| Theta | 0 | 90 | 0 | 0 | deg | |
| ORDINATE | | | | | | units |
| | Ymin | Ymax | VALmin | VALmax | | |
| Tn | 0 | 100 | 1.27759 | 91.3405 | % | |
| Tp | 0 | 0 | 0 | 0 | % | |
| Rn | 2 | 12 | 3.9208 | 10.8154 | % | |
| Rp | 0 | 0 | 0 | 0 | % | |
| R1 | 0 | 0 | 0 | 0 | % | |
| Apds | 0 | 0 | 0 | 0 | % | |
| A=1-T-R | 0 | 0 | 0 | 0 | / | |
| Tau, Rho, Rho1 | 0 | 100 | 0 | 100 | % | |
| DELTA-1 | 0 | 0 | 0 | 0 | deg | |
| PSI-1 | 0 | 0 | 0 | 0 | deg | |
| DELTA-2 | 0 | 0 | 0 | 0 | deg | |
| PSI-2 | 0 | 0 | 0 | 0 | deg | |
| DELTA-3 | 0 | 0 | 0 | 0 | deg | |
| PSI-3 | 0 | 0 | 0 | 0 | deg | |
| DELTA-4 | 0 | 0 | 0 | 0 | deg | |
| PSI-4 | 0 | 0 | 0 | 0 | deg | |
| MF | 0 | 1 | 0.00148169 | 1.3509 | / | |
| n | 0.5 | 2 | 1.47693 | 1.98592 | / | |
| k | 0 | 0.3 | 0.00117136 | 0.168283 | <input type="checkbox"/> log scale | |
| eps1 | 1.2 | 1.9 | 1.6606 | 2.9786 | / | |
| eps2 | 0 | 1 | 0.00422442 | 0.585682 | / | |
| graph | 6 | 0.5 | 3 | 0 | / | |

Read cursor on window = 1 wt: 0 (A) 0 (eV) Y: 0 ☐ Verbose

Load Spj! Save Spj! ito_ve001.1.Spj info: INDESIT ITO-4/1A Mag 2012

Load nk! Save nk! ito_ve001.3.nk info: INDESIT ITO-4/1A; Ibridone 19/gen/2017 Clear nk!

Figure 11: “Graph range” TAB.

3.6 Graph range TAB

The Graph range TAB (see Fig. 11) is dedicated to the graph window control.

On the top of this TAB, on the right of “ABSCISSA”, the checkbox “set eV scale” controls the abscissa: when checked the unit is eV, otherwise is Å. Please note that this choice is completely independent by the step used to re-sample measurements and file-*nk* loaded in the Valin TAB.

The Graph range TAB has 4 columns of fields; except for the last row, only the values in the first two columns can be edited, to set minimum and maximum values of the scale used in the different graphs. The values reported in 3rd and 4th columns are the minimum and maximum of the loaded data.

Only for the graph of the imaginary part of the complex refractive index the user can enable the logarithmic scale by ticking the box at the end of the row.

Differently from all the others, the last row has three editable fields (the fourth is not used) with the following graph parameters:

- width (inches)
- vertical to horizontal ratio
- line thickness.

To make the new values of these three graph features effective, the user has to save the project and restart the program.

For all the other settings, the opened graphical windows will be refreshed when the focus will go back to any another TAB.

4 Mini-guide to the characterization procedure

In order to facilitate the use of kSEMAW, this section describes a recommended sequence of operations / checks that allows one to obtain a reliable characterization of samples. Later, once the user becomes familiar with the software and above all with the topic, he will have the opportunity to define his own procedure, perhaps specific for a given family of samples.

- Check that the measured spectra have no artifacts (such as an abrupt discontinuity) and that the sum of transmittance and reflectance (measured under the same incidence angle) is below 100%.
- Load spectra (measurements) and file- nk into the Valin TAB and save the project. In the case of hemispherical measurements, tick the appropriate field. If necessary, specify the spectrum of the reference sample and tick the appropriate field to multiply the reflectance spectra for the reference one, during the data upload.
- Set the model in the Model TAB starting from the simplest hypothesis (substrate, homogeneous film, etc.).
- Surf to the Simulation TAB and plot the experimental measurements. To get an idea of the refractive index value, select “nk cte” from the nk-unknown menu and, by trial and error, try to reproduce the spectrum in a low absorption region (usually toward the NIR energy range). If necessary, adjust the thickness of an eventual thin film.
- Surf to the Graph-range TAB and set the ranges of n and k over which the numerical search for solutions has to be run. **Warning: the search intervals coincide with the n and k graphs scale!** If necessary, adjust the vertical axis scale of those plots.
- Surf to the Solution-tracking TAB and tick the measurements you intend to use in the numerical search; in the case of a thin film, it is recommended to start with only two spectra (typically transmittance and reflectance measured on the front side) because this allows one to more easily understand the types of discontinuities that will be eventually observed.
- Select a wavelength λ_0 towards the NIR (as an example wlMAX) taking care that it is not too close to an interference peak/valley. Launch the command “! Search in n-k space”. If the search range has been correctly set, two solution bands will be drawn; their intersection contains the sought solution. If not, adjust the search area in the space (n, k) until an intersection is found. Then enter the values n_{λ_0} and k_{λ_0} in the two fields below “@wlMAX”.
- Push the button “Set/Refresh graph!” and then “Search from wlMAX”. Solutions will be computed from the initial one and plotted in the graphs λ - n and λ - k . If “free from previous value” is the adopted strategy, when n goes out of the search area, the search is stopped and instructions are displayed in the terminal.
- **For substrates:**, once solutions over the full spectral range have been obtained, push the button “Store nk in”, and then “Save nk!” to save them permanently on

the hard disk with a suitable name. It is recommended to fill the field “info:” with the basic information that will help to remember the meaning of the files in the future.

For thin films: in order to obtain connected solutions, it will be necessary to carefully optimize the optical model, by adjusting the thickness and possibly introducing gradient / curvature and / or roughness. Once reasonably connected solutions are obtained, these have to be saved as described just above.

- Inevitably the solution trend in the λ - n space will present anomalies due to measurement errors and, in the case of thin films, to the intersections between solution branches. In order to obtain a more regular behaviour, the user should surf to Simulation TAB and set-up a fit option consisting of a suitable number of oscillators, preferably selected on the basis of physical criteria related to the material under investigation. By pressing “Plot exp. measures!” and then “Simulate!” the user can adjust all the parameters of the selected oscillators to get reasonable initial values.
- Surf to the IbridOne TAB, make all the parameters of interest of the previously configured fit option visible, enable a number of them for best fitting, push “Set/Refresh graphs !” and then “Fit n!” for launching the best-fit process. By pressing “Fit n and k!”, the best fit is also applied to k values. We recommend to start the best-fit with just a few enabled parameters, and then gradually include all the others to be optimized.
- From this point on the user can start the IbridOne procedure by pressing the button “Best Fit with IbridOne!”, provided that all the relevant parameters of the optical model (such as thickness, gradient, curvature ..) are made visible. Once again one should start the procedure by enabling just a few parameters, and then gradually include all the others in the optimization process. Once the result is satisfactory, push “! ibridOne with ERR and store nk in” for computing and storing solutions and errors. The final permanent saving on the hard disk can be done as explained above.

A Oscillators expressions

Up to now we have described the light propagation in multilayers using the wavelength λ and the refractive index $n - ik$ as independent variables. To describe the interaction of photons with matter it is instead more convenient to use the photon energy $E = h\nu = \hbar\omega = hc/\lambda$ and the relative permittivity $\epsilon_1 - i\epsilon_2$.

Refractive index and permittivity are both complex quantities connected by the equations

$$\epsilon_1 = n^2 - k^2, \quad \epsilon_2 = 2nk.$$

and inversely

$$n = \frac{1}{\sqrt{2}} \sqrt{\sqrt{\epsilon_1^2 + \epsilon_2^2} + \epsilon_1}, \quad k = \frac{1}{\sqrt{2}} \sqrt{\sqrt{\epsilon_1^2 + \epsilon_2^2} - \epsilon_1}. \quad (1)$$

Generally the theories for the light-matter interaction give simpler expressions for the permittivity. We here describe such expressions which will be numerically converted to refractive index values inside the code.

Optical data analysis is often performed by best-fitting the parameters of some functions modelling $n(E)$ and $k(E)$ or $\epsilon_1(E)$ and $\epsilon_2(E)$. Even if these functions may be in principle arbitrary, it is much more convenient that they possess a simple physical interpretation and satisfy the Kramers-Kronig relations.

The simplest functions are those representing the complex dielectric susceptibility $\tilde{\chi} = \chi_1 - i\chi_2$ associated to single resonant oscillators, obtained from both a classical (Drude-Lorentz oscillator) or a quantum approach. Dielectric susceptibility and permittivity are connected by the simple equation

$$\tilde{\epsilon} = \epsilon_1 - i\epsilon_2 = 1 + \tilde{\chi} = 1 + \chi_1 - i\chi_2. \quad (2)$$

In the current version, kSEMAW can model the dependence of the refractive index on wavelength $n(\lambda)$ with 7 different fit options; each option can be built using up to 20 oscillators belonging to the following 9 classes:

- Lorentz
- Quant-homo
- Quant-inhomo
- Flat
- Drude
- Direct Gap Cody
- Direct Gap Tauc
- Indirect Gap Cody
- Indirect Gap Tauc

Once the user sets a fit option, kSEMAW will calculate the total $\tilde{\epsilon}$ adding up the susceptibilities of all the selected oscillators: the *Flat* oscillator will take into account the “1” in Eq. 2. The complex refractive index will be then calculated using Eq. 1.

For each selected oscillator the user has to fill the parameter boxes. With the exception of *Flat* and *Drude* oscillators, the oscillators have 4 parameters: C , E_0 , D , K . Their meaning will be explained in the following description of each oscillator type.

A.1 Lorentz

The “Lorentz” oscillator is based on the classic Lorentz oscillator formulas [6]

$$\chi_1 = \frac{C(E_0^2 - E^2)}{(E_0^2 - E^2)^2 + (ED)^2}, \quad \chi_2 = \frac{KCED}{(E_0^2 - E^2)^2 + (ED)^2}$$

where $C = \frac{Nq^2\hbar^2}{m^*\epsilon_0}$ is the oscillator amplitude⁵, i.e. a constant [eV²] which multiplies both the real and the imaginary part of the susceptibility, E_0 is the resonance energy while D is the line width; these two last parameters are expressed in eV.

The K parameter multiplies the imaginary part only, representing another degree of freedom in the fitting procedure.

If $k \ll n$ these formulas give the approximate behaviour of $n(\lambda)$ described by the Sellmeier formula.

A.2 Homogeneous quantum oscillator

The “Quant-homo” oscillator is based on the simple quantum oscillator formulas [7] valid for the case of homogeneous broadening:

$$\chi_1 = \frac{C(E_0 - E)/D}{1 + [(E_0 - E)/D]^2}, \quad \chi_2 = \frac{KC}{1 + [(E_0 - E)/D]^2}.$$

The meaning of the four parameters C , E_0 , D , K is the same as in the previous case, but here C is dimensionless. The difference between Lorentz and quantum oscillators is shown in Fig. 12 where 1 was added to the susceptibility to get the permittivity.

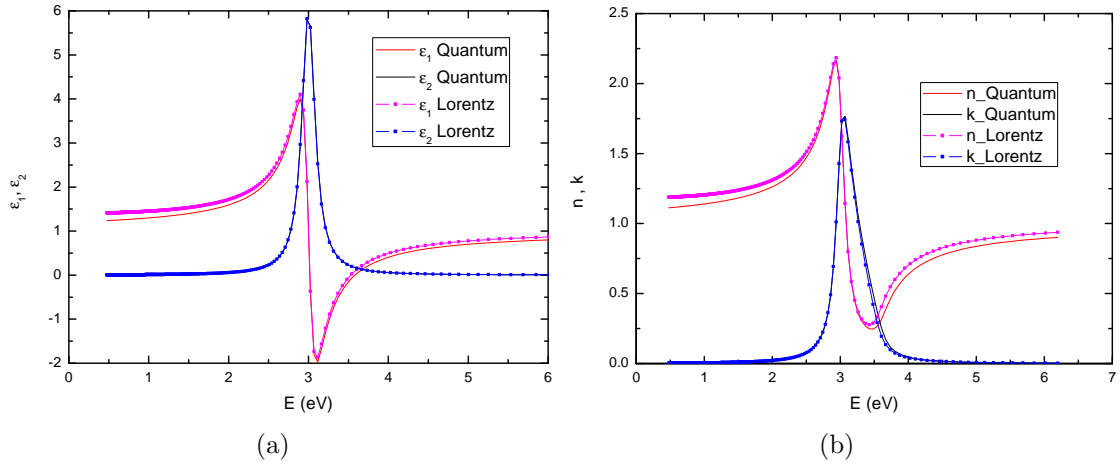


Figure 12: Behaviour of ϵ_1, ϵ_2 (a) and of n, k (b) for quantum ($C=6$, $E_0 = 3$ eV, $D=0.1$ eV) and Lorentz ($C=3.6$ eV², $E_0 = 3$ eV, $D=0.2$ eV) oscillators.

As reported in [8], the “Quant-homo” oscillator formula is obtained by neglecting a not-resonant term in the quantum treatment (otherwise a formula practically equivalent to the Lorentz oscillator would be obtained). As shown in Fig. 12 this approximation is excellent near the resonance energy while a small difference appears far away from it. On the other hand the simple and elegant equations obtained with this approximation allows one to obtain analytical expressions when the oscillator is used to make convolutions in materials with a continuous distribution of density of states.

⁵where N is the carrier density, q is the carrier charge, m^* is the carrier effective mass and ϵ_0 is the vacuum dielectric constant.

A.3 Inhomogeneous quantum oscillator

When the absorbing centres in a material cannot be considered as identical replicas, the absorption-line broadening is inhomogeneous. For example absorbing centres may be slightly different in a crystal because of the random presence of strain or proximity to other lattice defects and impurities that are randomly distributed or in a polycrystalline material because of the random orientations and sizes of the grains. The “Quant-inhomo” oscillator formula is therefore obtained by making the convolution between a homogeneous quantum oscillator and a Gaussian distribution centred in E_0 and with half width at half maximum (HWHM) equal to D [9]; the line width of the homogeneous quantum oscillator is assumed to be much lower than the Gaussian one.

A.4 Flat

The “Flat” oscillator is a simple constant term:

$$\epsilon_1 = C^2, \quad \epsilon_2 = 0.$$

It has to be noted that in this special case the C value is squared to obtain ϵ_1 so that C corresponds the refractive index offset generated by this “Flat” oscillator: $n = C + \dots$

NB: a “flat” oscillator with $C > 1$ must be always inserted into every option fit to take into account the vacuum permittivity ϵ_0 as well as the tail-contribute of some transitions at high energies, out of the investigated wavelength range, and not explicitly considered.

A.5 Drude

The “Drude” oscillator is based on the formulas which describe the response of a free electron gas:

$$\chi_1 = -\frac{E_0^2}{D^2 + E^2}, \quad \chi_2 = \frac{E_0^2 D}{E(D^2 + E^2)}.$$

In this case D is related to the carrier scattering time τ by $D = \hbar/\tau$ while E_0 is given by $E_0^2 = (\hbar^2 N q^2)/(m^* \epsilon_0)$ where N is the carrier density per unit volume and m^* is their effective mass. Please note that here C and K are not used.

Complex refractive index and complex dielectric constant as a function of energy are shown in Fig. 13. To obtain a reasonable permittivity a constant equal to 4 has been added to the susceptibility. This offset, generally called ϵ_∞ , is larger than 1 to take into account the tail-contribute of high energy oscillators, as explained previously.

An important energy value is the longitudinal plasma energy i.e. the energy for which $\epsilon_1 = 0$. This energy is given by $E_p^2 = E_0^2/\epsilon_\infty - D^2$ and it is located between the minimum and the flex in $n(E)$. Therefore we can shift the $n(E)$ minimum by changing E_0 , but this will also affect the behaviour at low energies. When E approaches zero, both n and k diverge. For $E \ll D$, $n \simeq k \simeq \sqrt{E_0^2/(2ED)}$.

In textbooks it is often stated that at short wavelengths the absorption coefficient increases like λ^2 , which is equivalent to say that $k(\lambda)$ increases like λ^3 . This approximated behaviour can be obtained from the relation $\epsilon_2 = \chi_2 = 2nk$ supposing that n is nearly constant. In this case, if $E \gg D$, we have that $k = E_0^2 D/(2nE^3)$.

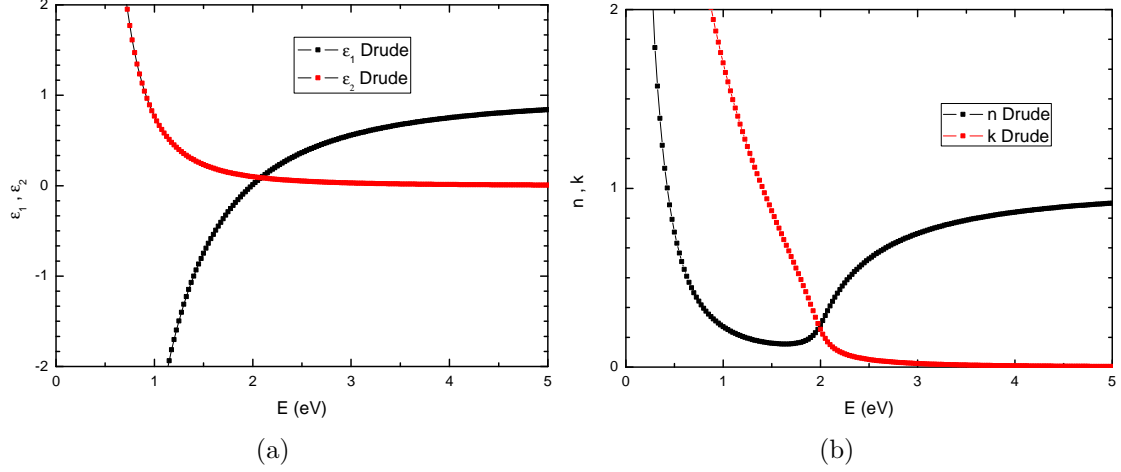


Figure 13: Behaviour of ϵ_1, ϵ_2 (a) and n, k (b) for a Drude oscillator ($E_0 = 1.57$ eV, $D = 0.2$ eV, $\epsilon_\infty = 4$).

This behaviour is visible in Fig. 14, showing $n(\lambda)$ and $k(\lambda)$, below 1000 nm; conversely for longer wavelengths the minimum in $n(\lambda)$ completely modifies the behaviour giving a nearly linear increase.

The Drude oscillator is typically used to fit the optical constants of TCOs. An example for a typical ITO is contained in ref. [10] where $E_p = 0.78$ eV, $\epsilon_\infty = 4$, $D = 0.2$ eV are found and therefore $E_0 = 1.57$ eV is deduced. If the carrier effective mass is known ($m^* = 0.35m_e$ for ITO [10]) the carrier concentration can be obtained from E_0 by using:

$$N(\text{cm}^{-3}) = E_0^2(\text{eV}) \frac{m^*}{m_e} 7.25 \cdot 10^{20};$$

with the previously given numbers we get $N = 6.25 \cdot 10^{20} \text{ cm}^{-3}$ for that material.

Moreover the optical mobility can be calculated from $D = \hbar/\tau$ using the equation $\mu = q\tau/m^*$. Numerically we have:

$$\mu\left(\frac{\text{cm}^2}{\text{Vs}}\right) = \frac{1.159}{D(\text{eV})m^*/m_e}$$

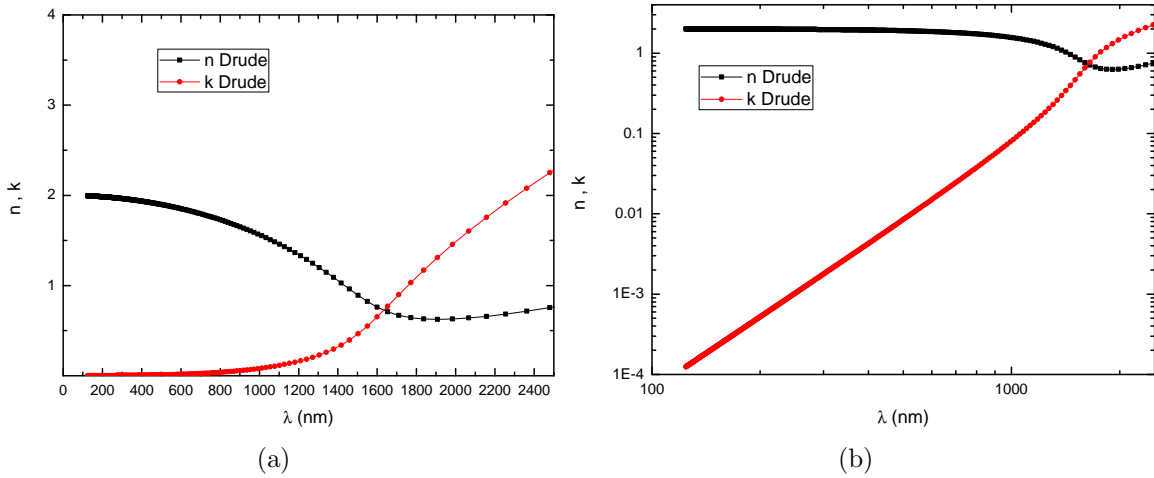


Figure 14: Linear (a) and double logarithmic (b) plot of n, k versus λ for a Drude oscillator ($E_0 = 1.57$ eV, $D=0.2$ eV, $\epsilon_\infty = 4$).

with the previously given numbers we get $\mu = 16.5 \text{ cm}^2/(\text{Vs})$ for that material.

A.6 Direct gap

The oscillators introduced up to now are unsuitable to describe the optical constants of systems with a continuous distribution of density of states such as semiconductors.

As a matter of fact the semiconductors theories reported in textbooks [11] usually derive $\epsilon_2 = \chi_2$ only and exclusively at energies near the fundamental gap. Furthermore the calculation is made by hypothesizing that the excited states have infinite lifetime, i.e. that every transition between two states may take place only by absorbing photons which energy is exactly equal to the difference of their energetic levels; the real part ϵ_1 is not explicitly calculated, but it can be obtained by means of the Kramers-Kronig relations. Since the Kramers-Kronig integrals have to be numerically computed (except for particular cases) that approach is not so convenient for best-fit procedures.

In kSEMAW analytical expressions for both χ_1 and χ_2 , satisfying the Kramers-Kronig relations and having a clear physical interpretation, are used. These expressions are obtained by performing the convolution between a suitable χ_2^{inf} calculated for infinite lifetime and the normalized complex $\tilde{\chi}_{qo}$ describing the response of a quantum oscillator:

$$\tilde{\chi}(E) = \int \chi_2^{inf}(E_r) \tilde{\chi}_{qo}(E_r - E) dE_r \quad (3)$$

The function $\tilde{\chi}_{qo}$ is given by the expression given before normalized by $C = 1/(\pi D)$ so that the integral of its imaginary part is equal to 1:

$$\tilde{\chi}_{qo}(E, E_r) = \frac{1}{\pi D} \left[\frac{(E_r - E)/D}{1 + [(E_r - E)/D]^2} - i \frac{1}{1 + [(E_r - E)/D]^2} \right] \quad (4)$$

where E_r is the resonance energy.

The result of the convolution can be expressed as analytical functions in a few simple but interesting cases discussed below.

In general χ_2^{inf} can be expressed as the product of the joint density of states $\rho(E)$ and a transition intensity $I(E)$ [12]:

$$\chi_2^{inf}(E) = I(E) \rho(E) \quad (5)$$

$I(E)$ contains the squared modulus of the matrix element of the electron-photon interaction Hamiltonian between the initial and final states. In the dipole approximation the Hamiltonian is proportional to the position operator but it can be written in an equivalent way also by using the momentum operator. A relation between the matrix elements of these two operators can be obtained by using commutator relations:

$$|\langle p \rangle|^2 = |\langle r \rangle|^2 \left(\frac{mE}{\hbar} \right)^2 \quad (6)$$

The energy dependence of $I(E)$ cannot be easily predicted and therefore it is assumed to be a constant if $|\langle r \rangle|^2$ is supposed to be independent of energy while it is assumed to be proportional to $1/E^2$ if $|\langle p \rangle|^2$ is supposed to be independent of energy. The constant $|\langle p \rangle|^2$ assumption was used by Tauc et al. [13] in the interpretation of the optical absorption of amorphous semiconductors leading to the well known "Tauc plot" method to derive the optical gap. The constant $|\langle r \rangle|^2$ assumption was later proposed by Cody

[14] again for the amorphous semiconductor case. These two alternatives can be used for crystalline materials also. For example in crystalline GaAs the energy dependence of the optical absorption above the bandgap is better described by the constant position matrix element [12] instead of by the more commonly hypothesized constant momentum matrix element.

For a crystalline semiconductor with direct allowed transitions between two parabolic bands separated by an energy gap E_0 , $\rho(E)$ can be written as [11]:

$$\rho(E) = C_r(E - E_0)^{1/2} \quad (7)$$

This monotonically increasing expression for $\rho(E)$ is obviously valid only for energies slightly larger than the gap. For higher energy values $\rho(E)$ can show a rather complex behavior but it also has a high energy limit determined by the extension of the valence and conduction bands. At the gap energy (E_0) and at this high energy limit (E_3) the $\rho(E)$ has two "critical points" called $M0$ and $M3$ where it goes to zero following a square root behavior [11].

The simplest expression valid for every energy which has the correct square root behaviour near E_0 and E_3 is:

$$\rho(E) = C_r \sqrt{(E - E_0)(E_3 - E)} \quad (8)$$

By using this expression and the "Cody's approximation" the χ_2^{inf} also has the same form:

$$\chi_{2-dir-Cody}^{inf}(E) = C \sqrt{(E - E_0)(E_3 - E)} \quad (9)$$

Equation 9 can be considered as an acceptable approximation for $\chi_2^{inf}(E)$ in the case of a direct gap material with position matrix element independent of energy and with infinite lifetime (see Fig. 15 a).

On the other hand in Tauc's approximation, the momentum matrix element is as considered as independent of energy; therefore as previously discussed an additional factor $1/E^2$ has to be inserted in the formula (see Fig. 15 b):

$$\chi_{2-dir-Tauc}^{inf}(E) = C \frac{\sqrt{(E - E_0)(E_3 - E)}}{E^2} \quad (10)$$

Other types of critical points do exist ($M1$ and $M2$) in the $\rho(E)$ [11], but they are not yet included among the fitting functions of kSEMAW.

The expressions obtained by performing the convolution between the χ_2^{inf} and the normalized complex $\tilde{\chi}_{qo}$ in these two cases are:

Direct gap Cody:

$$\begin{aligned} \chi_{1-dir-Cody}(E) &= \frac{CD}{2} \left\{ a + b - 2(a^2 + 1)^{1/4}(b^2 + 1)^{1/4} \cos \left[\frac{1}{2} \arctan \left(\frac{1}{a} \right) + \frac{1}{2} \arctan \left(\frac{1}{b} \right) \right] \right\} \\ &= \frac{CD}{2} \left[a + b - 2\Re \left(\sqrt{a + i} \sqrt{b + i} \right) \right] \quad (11) \end{aligned}$$

$$\begin{aligned} \chi_{2-dir-Cody}(E) &= -CD \left\{ 1 + (a^2 + 1)^{1/4}(b^2 + 1)^{1/4} \sin \left[\frac{1}{2} \arctan \left(\frac{1}{a} \right) + \frac{1}{2} \arctan \left(\frac{1}{b} \right) \right] \right\} \\ &= -CD \left[1 - \Im(\sqrt{a + i} \sqrt{b + i}) \right] \quad (12) \end{aligned}$$

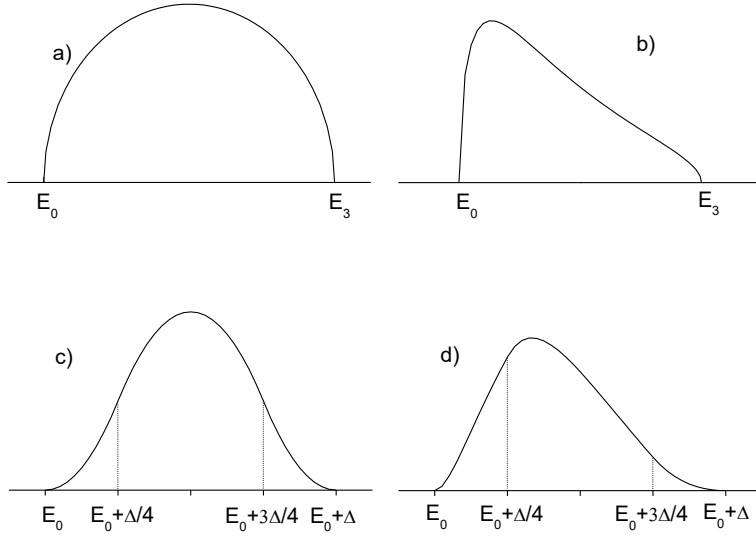


Figure 15: χ_2^{inf} for infinite lifetime semiconductor and: a) direct gap under Cody's approximation b) direct gap under Tauc's approximation, c) indirect gap under Cody's approximation d) indirect gap under Tauc's approximation

where $a = \frac{E_0 - E}{D}$ and $b = \frac{E_3 - E}{D}$.

Direct gap Tauc

$$\chi_{1-dir-Tauc}(E) = \frac{C}{2D}$$

$$\Re \left\{ \frac{1}{2(D-iE)} \left(2iD + 2E - 2\sqrt{E_0 E_3} - (i-1)\sqrt{2}\sqrt{D-i(E-E_0)}\sqrt{-iD-E+E_3} \right) + \right.$$

$$\left. \frac{1}{2(D+iE)} \left(-2iD + 2E - 2\sqrt{E_0 E_3} + (i+1)\sqrt{2}\sqrt{D+i(E-E_0)}\sqrt{iD-E+E_3} \right) + \right.$$

$$\frac{E(D-iE)^2\sqrt{D+i(E-E_0)}\sqrt{D+i(E-E_3)}}{(D^2+E^2)^2} +$$

$$\frac{E(D+iE)^2\sqrt{D-i(E-E_0)}\sqrt{D-i(E-E_3)}}{(D^2+E^2)^2} -$$

$$\left. \frac{ED(D^2(E_0+E_3) + E(-4E_0E_3 + E(E_0+E_3)))}{(D^2+E^2)^2\sqrt{E_0E_3}} \right\} \quad (13)$$

$$\chi_{2-dir-Tauc}(E) = CD$$

$$\Re \left\{ - \left[(D-iE)^2\sqrt{D+i(E-E_0)}\sqrt{D+i(E-E_3)} \right] / \left(2D(D^2+E^2)^2 \right) - \right.$$

$$\left. \left[(D+iE)^2\sqrt{D-i(E-E_3)}\sqrt{D-i(E-E_0)} \right] / \left(2D(D^2+E^2)^2 \right) + \right.$$

$$\left. \frac{D[D^2(E_0+E_3) + E(-4E_0E_3 + E(E_0+E_3))]}{(2D(D^2+E^2)^2\sqrt{E_0E_3})} \right\} \quad (14)$$

It must be noted that the input parameter K is used to transfer through the code the information about the bandwidth: $K = E_3 - E_0$.

A.7 Indirect Gap

In the two previous cases we considered direct transitions i.e. transitions where the excitation takes place with the absorption of a single photon. In this case the crystalline momentum of the electron excited in the conduction band must be practically equal to the momentum of the electron in the valence band.

Different formulas must be used for materials where the fundamental gap is due to indirect transitions: in this case the excitation process includes the absorption or the emission of a phonon necessary to allow transitions between electronic states with different crystalline momentum. The absorption/emission of phonon remove the momentum conservation constraint and therefore for indirect transitions $\rho(E)$ is proportional to the convolution of the density of states of the two bands. In amorphous semiconductors also the momentum conservation is not required because the disorder destroy translational symmetry and momentum is no more a good quantum number. It follows that oscillators for indirect transitions in crystalline semiconductors can be used to fit the optical constants of amorphous semiconductors too.

Unfortunately the convolution integral of two finite bands has no analytical expression even in the simplest case where both the valence and the conduction band have the form given by Eq. 8. On the other hand it is well known that the convolution between two square root densities of states gives a function which increases parabolically above the gap. Therefore an empirical approximated expression can be obtained by joining two parabolic edges with a parabolic maximum, getting Cody's approximation (see Fig. 15 c):

$$\chi_{2-ind-Cody}^{inf}(E) = \frac{16C}{\Delta^2}(E - E_0)^2 \quad \text{if } E_0 < E < E_0 + \Delta/4 \quad (15)$$

$$\chi_{2-ind-Cody}^{inf}(E) = C \left\{ 2 - \frac{16}{\Delta^2} [E - (E_0 + \Delta/2)]^2 \right\} \quad \text{if } E_0 + \frac{\Delta}{4} < E < E_0 + \frac{3\Delta}{4} \quad (16)$$

$$\chi_{2-ind-Cody}^{inf}(E) = \frac{16C}{\Delta^2} [E - (E_0 + \Delta)]^2 \quad \text{if } E_0 + \frac{3\Delta}{4} < E < E_0 + \Delta \quad (17)$$

where E_0 is the gap energy and Δ is the absorption band width.

In the Tauc's approximation the expressions are obviously (see Fig. 15 d):

$$\chi_{2-ind-Tauc}^{inf}(E) = \frac{16C}{\Delta^2 E^2} (E - E_0)^2 \quad \text{if } E_0 < E < E_0 + \Delta/4 \quad (18)$$

$$\chi_{2-ind-Tauc}^{inf}(E) = \frac{C}{E^2} \left\{ 2 - \frac{16}{\Delta^2} [E - (E_0 + \Delta/2)]^2 \right\} \quad \text{if } E_0 + \frac{\Delta}{4} < E < E_0 + \frac{3\Delta}{4} \quad (19)$$

$$\chi_{2-ind-Tauc}^{inf}(E) = \frac{16C}{\Delta^2 E^2} [E - (E_0 + \Delta)]^2 \quad \text{if } E_0 + \frac{3\Delta}{4} < E < E_0 + \Delta \quad (20)$$

As for the direct gap case, both the complex permittivity components can be obtained by the convolution between these parabolic terms and the quantum oscillator $\tilde{\chi}_{qo}$. The analytical χ_2 expressions are:

Indirect gap-Cody

$$\begin{aligned} \chi_{1-ind-Cody}(E) = & C \{ 2IC_{Re}^{Cody}(E, E_0 + 3\Delta/4) - 2IC_{Re}^{Cody}(E, E_0 + \Delta/4) + \\ & 16/\Delta^2 [+ I2_{Re}^{Cody}(E, E_0, E_0 + \Delta/4) - I2_{Re}^{Cody}(E, E_0, E_0) \\ & - I2_{Re}^{Cody}(E, E_0 + \Delta/2, E_0 + 3\Delta/4) + I2_{Re}^{Cody}(E, E_0 + \Delta/2, E_0 + \Delta/4) \\ & + I2_{Re}^{Cody}(E, E_0 + \Delta, E_0 + \Delta) - I2_{Re}^{Cody}(E, E_0 + \Delta, E_0 + 3\Delta/4)] \} \end{aligned} \quad (21)$$

where:

$$IC_{Re}^{Cody}(E, E_r) = \frac{1}{\pi D} \int \frac{[(E_r - E)/D] dE_r}{1 + [(E_r - E)/D]^2} = \frac{1}{2\pi} \ln [D^2 + (E - E_r)^2] \quad (22)$$

$$I2_{Re}^{Cody}(E, E_0, E_r) = \frac{1}{\pi D} \int \frac{(E_r - E_0)^2 [(E_r - E)/D] dE_r}{1 + [(E_r - E)/D]^2} = \frac{1}{2\pi} \left\{ (E_r - E)(3E - 4E_0 + E_r) + 4D(E - E_0) \arctan\left(\frac{E - E_r}{D}\right) + [(E - E_0)^2 - D^2] \ln [D^2 + (E - E_r)^2] \right\} \quad (23)$$

$$\begin{aligned} \chi_{2-ind-Cody}(E) = C \{ & 2IC_{Im}^{Cody}(E, E_0 + 3\Delta/4) - 2IC_{Im}^{Cody}(E, E_0 + \Delta/4) + \\ & 16/\Delta^2 [+ I2_{Im}^{Cody}(E, E_0, E_0 + \Delta/4) - I2_{Im}^{Cody}(E, E_0, E_0) \\ & - I2_{Im}^{Cody}(E, E_0 + \Delta/2, E_0 + 3\Delta/4) + I2_{Im}^{Cody}(E, E_0 + \Delta/2, E_0 + \Delta/4) \\ & + I2_{Im}^{Cody}(E, E_0 + \Delta, E_0 + \Delta) - I2_{Im}^{Cody}(E, E_0 + \Delta, E_0 + 3\Delta/4)] \} \end{aligned} \quad (24)$$

where:

$$IC_{Im}^{Cody}(E, E_r) = \frac{1}{\pi D} \int \frac{dE_r}{1 + [(E_r - E)/D]^2} = -\frac{1}{\pi} \arctan\left(\frac{E - E_r}{D}\right) \quad (25)$$

$$I2_{Im}^{Cody}(E, E_0, E_r) = \frac{1}{\pi D} \int \frac{(E_r - E_0)^2 dE_r}{1 + [(E_r - E)/D]^2} = \frac{1}{\pi} \left([D^2 + (E - E_0)^2] \arctan\left(\frac{E - E_r}{D}\right) + D \{ E_r - E + (E - E_0) \ln [D^2 + (E - E_r)^2] \} \right) \quad (26)$$

Indirect gap-Tauc

$$\begin{aligned} \chi_{1-ind-Tauc}(E) = C \{ & 2IC_{Re}^{Tauc}(E, E_0 + 3\Delta/4) - 2IC_{Re}^{Tauc}(E, E_0 + \Delta/4) + \\ & 16/\Delta^2 [+ I2_{Re}^{Tauc}(E, E_0, E_0 + \Delta/4) - I2_{Re}^{Tauc}(E, E_0, E_0) \\ & - I2_{Re}^{Tauc}(E, E_0 + \Delta/2, E_0 + 3\Delta/4) + I2_{Re}^{Tauc}(E, E_0 + \Delta/2, E_0 + \Delta/4) \\ & + I2_{Re}^{Tauc}(E, E_0 + \Delta, E_0 + \Delta) - I2_{Re}^{Tauc}(E, E_0 + \Delta, E_0 + 3\Delta/4)] \} \end{aligned} \quad (27)$$

where:

$$IC_{Re}^{Tauc}(E, E_r) = \frac{1}{\pi D} \int \frac{[(E_r - E)/D] dE_r}{E_r^2 [1 + [(E_r - E)/D]^2]} = \frac{1}{2\pi(D^2 + E^2)^2} \left\{ -4DE \arctan\left(\frac{E - E_r}{D}\right) + \frac{2E(D^2 + E^2)}{E_r} + (E^2 - D^2) \ln\left(\frac{D^2 + (E - E_r)^2}{E_r^2}\right) \right\} \quad (28)$$

$$\begin{aligned}
I2_{Re}^{Tauc}(E, E_0, E_r) &= \frac{1}{\pi D} \int \frac{(E_r - E_0)^2 [(E_r - E)/D] dE_r}{E_r^2 [1 + [(E_r - E)/D]^2]} = \\
&\frac{1}{2\pi(D^2 + E^2)^2} \left\{ 4DE_0(D^2 + E^2 - EE_0) \arctan\left(\frac{E - E_r}{D}\right) \right. \\
&+ [D^4 + E^2(E - E_0)^2 + D^2(2E^2 - 2EE_0 - E_0^2)] \ln(D^2 + (E - E_r)^2) \\
&\left. + 2E_0 \left[\frac{E(D^2 + E^2)E_0}{E_r} + (E^2(2E - E_0) + D^2(2E + E_0)) \ln(E_r) \right] \right\} \quad (29)
\end{aligned}$$

$$\begin{aligned}
\chi_{2-ind-Tauc}(E) &= C \{ 2IC_{Im}^{Tauc}(E, E_0 + 3\Delta/4) - 2IC_{Im}^{Tauc}(E, E_0 + \Delta/4) + \\
&16/\Delta^2 [+ I2_{Im}^{Tauc}(E, E_0, E_0 + \Delta/4) - I2_{Im}^{Tauc}(E, E_0, E_0) \\
&- I2_{Im}^{Tauc}(E, E_0 + \Delta/2, E_0 + 3\Delta/4) + I2_{Im}^{Tauc}(E, E_0 + \Delta/2, E_0 + \Delta/4) \\
&+ I2_{Im}^{Tauc}(E, E_0 + \Delta, E_0 + \Delta) - I2_{Im}^{Tauc}(E, E_0 + \Delta, E_0 + 3\Delta/4)] \} \quad (30)
\end{aligned}$$

where:

$$\begin{aligned}
IC_{Im}^{Tauc}(E, E_r) &= \frac{1}{\pi D} \int \frac{dE_r}{E_r^2 [1 + [(E_r - E)/D]^2]} = \\
&-\frac{1}{\pi(D^2 + E^2)^2} \left\{ (E^2 - D^2) \arctan\left(\frac{E - E_r}{D}\right) + D \left[\frac{(D^2 + E^2)}{E_r} + E \ln\left(\frac{D^2 + (E - E_r)^2}{E_r^2}\right) \right] \right\} \quad (31)
\end{aligned}$$

$$\begin{aligned}
I2_{Im}^{Tauc}(E, E_0, E_r) &= \frac{1}{\pi D} \int \frac{(E_r - E_0)^2 dE_r}{E_r^2 [1 + [(E_r - E)/D]^2]} = \\
&-\frac{1}{\pi(D^2 + E^2)^2} \left\{ [D^4 + E^2(E - E_0)^2 + D^2(2E^2 - 2EE_0 - E_0^2)] \arctan\left(\frac{E - E_r}{D}\right) \right. \\
&\left. + DE_0 \left[\frac{(D^2 + E^2)E_0}{E_r} + (D^2 + E^2 - EE_0) \ln\left(\frac{E_r^2}{D^2 + (E - E_r)^2}\right) \right] \right\} \quad (32)
\end{aligned}$$

B Some useful rules of good practice

During my experience developed over thirty years, I have often observed that neophytes tend to underestimate the problems associated with spectrophotometric measurements; these problems become even greater when one needs the absolute values of the measurement, as requested by kSEMAW.

Without any claim of exhaustiveness, I list below some rules that user should take care to fulfil in order to avoid the most common mistakes.

B.1 n, k of the substrate

The most common error in characterizing thin film devices is to neglect the preliminary characterization of the substrate. As a matter of fact, although for a given type of material the real part of the refractive index is fairly constant over different specimens, and well compatible with the values reported in literature, the same cannot be said for the extinction coefficient: in the nearness of the absorption edges, such as the UV transmittance cutoff for glass and quartz, the user should not be surprised to find differences much greater than the measurement error, even among substrates belonging to the same batch! Thus if one intends to analyse a series of samples, the preliminary check about the homogeneity of the available substrates and, if necessary, the selection of a group with same features, are mandatory. In order to properly characterize thin film specimens, the loading in the Valin TAB of the right file- nk is essential, otherwise the found solutions will be subject to more or less evident artefacts.

B.2 Reflectance reference

Unless reflectance is measured by means of an absolute accessory, a reference specimen is required. A very common error is to measure the hemispherical reflectance of a sample with good specular characteristics by using a diffusive reference, like the cover of the port supplied with the integrating sphere. This will lead to artefacts induced by the dependence, albeit weak, of the response of an integrating sphere from the emission angle, with respect to the optical axis, of the transmitted/reflected rays.

In the case of relative specular reflectance accessories, a frequent error is to overlook the dependence of the response on the distance between the most reflective surface and the reference plane on which the sample lays (for example three tips). As an example, *first-face* mirrors (i.e. with reflective treatment on the *front face*) should not be measured using *second-face* reference mirrors; in this case the error will be larger for reference mirrors with thicker substrates.

Consequently, the following golden rule must be respected: **always use a reference sample as similar as possible to the sample to be characterized: specular for specular, diffusive for diffusive, etc ..**

When a certified sample suitable for own needs is purchased, a secondary reference sample, even homemade, should be obtained and used in everyday measurements.

If mirrors/specimens are placed on a reference plane (i.e. the exit port of the integrating sphere), it is strongly recommended to make a frame spacer in which to insert the mirror, in order to avoid the direct contact between reflective and reference surfaces.

B.3 Prismatic sample

A sample with not perfectly parallel faces, like a prism, induces the deviation of the beam passing through it; in reflection instead it will give rise to two diverging beams.

The prismatic angle of the sample can be quantitatively assessed using a laser beam; otherwise the user should simply observe by eye the image reflected from the sample surface, of an object with well-defined edges, such as a neon lamp.

Except for the case of integrating spheres, the transmitted (reflected) beam(s) will impact the sensitive area of the detector in different sites (with respect to the calibration/baseline measurement); sometimes part of the beam(s) will fall out the detector; all this will significantly affect the measured value. In order to evaluate the entity of this problem, the user should observe the eventual variation of the signal obtained by rotating the sample around the optical axis of the instrument.

There are two solutions to this problem: i) use an integrating sphere; ii) use an integrating sphere just like a sensor in specular/direct measurements. The last solution requires that the spectrophotometer can be simultaneously equipped with an integrating sphere and a specular reflectance accessory; as for the transmittance, it will be enough to place the sample at an appropriate distance from the entry port of the integrating sphere.

B.4 Masks for small area samples

Samples made in research laboratories often offer a useful surface which is smaller than the section of the measurement beam. Unless the focusing optic of the instrument is changed, the easiest solution is the reduction of the spot size of the beam by means of a mask (diaphragm). In applying this solution, however, the following precautions must be taken:

- provide a mechanical system able to ensure the perfect repositioning of the mask each time it is removed, for example to place the sample after the baseline measurement
- arrange the mask **before** the sample along the beam path, for both transmittance and reflectance measurements
- in the case of hemispherical reflectance, in addition to performing the baseline and the measurement of the sample, the contribution of the mask must also be considered by performing a third scan without placing neither the sample nor the reference. This spectrum has to be subtracted from both the baseline and the sample spectrum, since the final value is given from by their ratio

B.5 Irregular thickness of the thin film

Another feature that is often observed on thin film samples made in research laboratories is a marked non-uniformity of the thickness. The consequence is the imperfect correspondence between the positions of the maxima and minima of the interference fringes in the reflectance and transmittance spectra of thin film.

The solution is to mark the sample and arrange it in such a way that the spot of the measuring beam, having a typical banana shape, impinges on the same area of the sample for all measurements.

B.6 Scan speed and integration time

Currently the most common UV-VIS-NIR spectrophotometers belong to the dispersive type. Unlike those belonging to the FTIR type (Fourier transform) commonly used for measurements in the IR region, in dispersion instruments the acquisition of the spectrum is obtained by changing the wavelength of the measure beam step by step; this implies a rather long acquisition time. So the neophyte, to hurry up the measurement, is inclined to select the highest speeds allowed by the software of the instrument (for example 480 nm/min), without evaluating the possible consequences: as a matter of fact in the case of spectra with sharp variations, such as the case of the transmittance UV cutoff of glass substrates or the interference fringes of thin film of sufficient thickness, the measured spectrum will be distorted both by the smoothing of maxima and minima (reduction of the peak-valley amplitude), and by the shift of the transients to UV, if scanning speed and instrument integration time are not well balanced. The latter artefact is caused by the reading delay combined with the scan direction of the selected range, from the maximum wavelength to the minimum one.

The presence of such artefacts can be verified by comparing the value of a static measurement reading (at a fixed wavelength), with the corresponding value in the spectrum, dynamically acquired. If the difference is greater than the measurement error, a better compromise between scanning speed and integration time has to be found.

Whenever a session of measures is undertaken on a different type of samples, careful analysis of this critical point is required.

B.7 Jump at the reticle-detector change

A sharp jump is frequently observed in the spectra obtained with dispersion instruments, at the wavelength at which reticle and detector are changed (typically 860 nm). Normally this phenomenon is less marked if an integrating sphere is used.

To overcome this problem it is necessary to balance the width of the slits (kept to a constant value in the UV-VIS region) with the electronic gain of the sensor used in the NIR. Sometimes it can be useful to modify the change wavelength, so as to make the intensity of the measurement signal more similar on both sides.

B.8 Misaligned spectrophotometer

A periodical check of the optical alignment of the spectrophotometer is strongly recommended. This operation requires a good experience of optical beam manipulation by the user. Otherwise a technical intervention is advisable or at least the supervision by a more experienced colleague.

The main check is to verify that the two beams (measure and reference) are well aligned both in and downstream of the sample holder compartment. Some software are equipped with tools for alignment diagnostics and sometimes self-optimizing hardware.

In my experience, the most serious and frequent episodes occur with integrating spheres, especially when they are frequently disassembled and reinstalled. In this case, by setting the instrument on white or green light, in dark-room conditions, the operator must verify that the beams pass in the centre of the entrance and exit ports. In case of imperfections, the return mirrors upstream to the sphere have to be adjusted.

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