



kSEMAWc software

**Spectrophotometric (SP),
Ellipsometric (ELI) and
photothermal deflection spectroscopy (PDS)
Measurements
Analysis Workbench**

k stands for the use of Qt libraries
c stands for full C++ language

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Summary

Part I - what is kSEMAWc intended for?

Part II - some software details:

- Language and libraries
- Where to find it?
- Installation

Part III – How to use it?

Part I : what is it for?

kSEMAWc deals with optical devices

- composed by layers (from 1 to 9) of
- homogeneous or not (EMA, graded index, ect.) materials
- thin ($d \leq \frac{\lambda^2}{\Delta\lambda}$) or thick,
- with plane and parallel interfaces,
- eventually, with moderate roughness ($\sigma \ll \lambda$)

Part I : what can it do?

kSEMAWc can:

- 1) Simulate spectrophotometric, ellipsometric, PDS spectra

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Part I : what can do?

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- 1) Simulate** spectrophotometric, ellipsometric, PDS spectra
- 2) Calculate** complex refractive index ($n - i k$) and thickness of a given thin layer, when the surrounding layers are known
- 3) Evaluate** mean value of Transmittance / Reflectance weighted on a given international or customized spectrum (D65, ASTM-G173, etc.)

Part I : what can do?

kSEMAWc can:

- 1) Simulate** spectrophotometric, ellipsometric, PDS spectra
- 2) Calculate** complex refractive index ($n - i k$) and thickness of a given thin layer, when the surrounding layers are known
- 3) Evaluate** mean value of Transmittance / Reflectance weighted on a given international or customized spectrum (D65, ASTM-G173, etc.)
- 4) Predict** Transmittance / Reflectance once a realistic or an equivalent model of the optical device has been set

Part II : some details



Language: full C++ (since v1.0.0)

Graphical User Interface: based on Qt library

Plots: based on Qwt library

Non linear least square: C/C++ MINPACK library, for Levenberg-Marquardt algorithm

Distribution: free open source under GNU v3 license

Downloadable from

<https://github.com/mmonty1960/ksemaw>



mmonty1960 / ksemaw

Type / to search



Code

Issues 2

Pull requests

Actions

Projects

Wiki

Security

Insights

Settings



ksemaw

Public

Unpin

Unwatch 1



Fork

0



Star

2

master



Go to file



Code

mmonty1960 v2.6

adca841 · 2 minutes ago

31 Commits

Workspace

v2.6

2 minutes ago

LICENSE.txt

version 0.9.6

3 years ago

OpenResEu_ksemaw_V2.pdf

v2.6

3 minutes ago

README.md

v2.6

3 minutes ago

gsl-2.7.zip

ksemawc-v2.1

7 months ago

ksemawc_WinExecLauncher.bat

version 1.0.0

2 years ago

manuale_ksemawc_V2.5.pdf

v2.5

2 months ago

README

GPL-3.0 license



ksemaw_v2.6

About

kSEMAW: a workspace for the analysis of Spectrophotometric (SP), Ellipsometric (ELI) and Photothermal Deflection Spectroscopy (PDS) measurements

Readme

GPL-3.0 license

Activity

2 stars

1 watching

0 forks

Releases

11

v2.6 Latest

yesterday

+ 10 releases

Packages

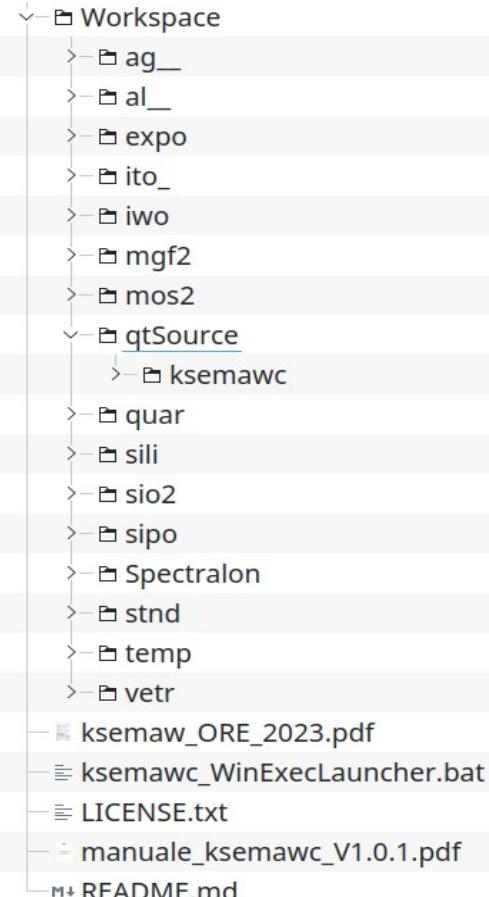
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Part II : the Workspace

Please note: users are asked to download the whole **Workspace**

folder, containing:

- source files
- configuration files
- exemplary data files
- MS Windows executable
and
- MS launcher
- user-manual
- ORE paper with some use cases



Option #1: compilation of source files

- OS: Linux, MS Windows, Mac (not tested)
- For MS Windows, preliminary installation of MinGW
- Libraries: Qt, Qwt, C/C++MINPACK
- Qt Creator (IDE): load ksemawc.pro and compile

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Option #2: only in MS Windows

Click on

ksemawc_WinExecLauncher.bat

Part III : please note

Important points:

- kSEMAWc works embedded in the Workspace folder
- All data files concerning a given optical device should be named with a unique code, adding suitable extensions (see the manual)
- Since version 1.0.0, kSEMAWc offers 3 different approaches for evaluating the unknown complex refractive index:
 - 1) **Exhaustive Numerical search** in λ -n space
 - 2) **Standard Fit** method
 - 3) **IbridOne** method (best-fit of R / Ψ with n modeled by oscillators, and k computed to reproduce T spectrum)

Part III : GUI and terminal



ksemawc

Valin Model Simulation Numerical Search Data Fit Graph Range

nk data keep k>=0 when loaded

Load nk_1	vetr/bk071.1	<input type="button" value="Clear"/>	vetrino SUPERFROST nk da Autos 27/apr/2012	3000	25000
Load nk_2	vetr/bk071.2	<input type="button" value="Clear"/>	Vetrino Superfrost; nk Ibridone; 27/apr/2012	3000	25000
Load nk_3	ito/_ve001.4	<input type="button" value="Clear"/>	INDESIT ITO-4/1A; IbrdiOne 22/nov/2022	3000	25000
Load nk_4	mate/aa999.9	<input type="button" value="Clear"/>			
Load nk_5	mate/aa999.9	<input type="button" value="Clear"/>			
Load nk_6	mate/aa999.9	<input type="button" value="Clear"/>			
Load nk_7	mate/aa999.9	<input type="button" value="Clear"/>			
Load nk_8	mate/aa999.9	<input type="button" value="Clear"/>			

Select Sample: ito/_ve001

Spectrophotometric measurements: Tp & Rp Theta_inc (deg) s-polarized

Error: DBase/Base DRRef/Ref ErrReading

<input checked="" type="checkbox"/> Tnorm	v1	<input type="button" value="▼"/>	ITO 4/1-A	2500	25000
<input type="checkbox"/> Tpol		<input type="button" value="▼"/>			
<input checked="" type="checkbox"/> Rnorm	v1	<input type="button" value="▼"/>	ITO4_1_A	2500	25000
<input type="checkbox"/> Rpol		<input type="button" value="▼"/>			
<input type="checkbox"/> R1norm		<input type="button" value="▼"/>			
<input type="checkbox"/> Apds		<input type="button" value="▼"/>			

hemispherical measurements multiply Rn, Rp, R1 by the reference mirror RIF08_since_13_December_2011

Ellipsometric measurements force resampling to cross experimental data

<input type="checkbox"/> ELI-1	<input type="button" value="▼"/>				
<input type="checkbox"/> ELI-2	<input type="button" value="▼"/>				
<input type="checkbox"/> ELI-3	<input type="button" value="▼"/>				
<input type="checkbox"/> ELI-4	<input type="button" value="▼"/>				

Wavelength range (Angstrom) From to 4.133->0.496 eV N. Points resample with eV step Manual setting of Graph WL-Range Verbose

ito/_ve001.1.Spj info: INDESIT: ITO-4/1A Mag 2012

ito/_ve001.4.nk info: INDESIT ITO-4/1A; IbrdiOne 22/nov/2022

ksemawc : ksemawc — Konsole

Marco@MM-hp2440 ~\$./ksemawc

Program C++ KSEMAW
Spectro-Ellipsometric Measurement Analysis Workbench
(spectrophotometric, ellipsometric and PDS)
version 2.6 8 January 2024
Main author: Marco Montecchi, ENEA (Italy)
email: marco.montecchi@enea.it
Porting to Windows and advanced oscillators by
Alberto Mittiga, ENEA (Italy)
email: alberto.mittiga@enea.it

pathroot: /home/marco/Workspace/
-> RefMir #1 -> al/_RIF05corr.txt
-> RefMir #2 -> al/_RIF06before5Dic1994corr.txt
-> RefMir #3 -> al/_RIF06after5Dic1994corr.txt
-> RefMir #4 -> al/_RIF05after18March1996corr.txt
-> RefMir #5 -> al/_rio08.v2.rn
-> RefMir #6 -> al/_rio08.v3.rn
-> RefMir #7 -> al/_rifPVenea.v1.rn
-> RefMir #8 -> Spectralon/LabspherePTFE8715.txt
-> StdSpectrum #0: VIS_10_wl (Glass in building) -> stdn/media.1
-> StdSpectrum #1: VIS_30_wl (Glass in building) -> stdn/media.2
-> StdSpectrum #2: VIS_D65 (Glass in building) -> stdn/media.3
-> StdSpectrum #3: solar_10_wl (Glass in building) -> stdn/media.4
-> StdSpectrum #4: solar_global_radiation (Glass in building) -> stdn/media.5
-> StdSpectrum #5: DNI_100_wl direct normal radiation -> stdn/media.6
-> StdSpectrum #6: PWO_scintillation -> stdn/pwtdr.1
-> StdSpectrum #7: PWO_scint*APDqe -> stdn/pwige.1
-> StdSpectrum #8: IEC_60904-3 -> stdn/IEC60904b3Step5nm.txt
-> StdSpectrum #9: ASTM_G173 solar normal direct radiation AM=1.5 -> stdn/ASTMG173SP.txt
-> StdSpectrum #10: ISO_9050 solar global radiation AM=1.5 -> stdn/ISO9050.txt
-> StdSpectrum #11: ISO_9845-1 solar normal direct radiation AM=1.5 -> stdn/ISO9845b1.txt
-> StdSpectrum #12: E_891 solar normal direct radiation AM=1.5 -> stdn/E891.txt
setting-file exists! /home/marco/.config/ksemawc/ksemawc.conf
-> SaveSetting (with option iCall=-1) to /home/marco/Workspace/temp/default.1.Spj
-> LoadProject
-> ReadSetting from /home/marco/Workspace/ito/_ve001.1.Spj
date: 2023-06-14 14:53:55
The project version is up-to-date
-> Setnk(1) with fnk[1]=/home/marco/Workspace/vetr/bk071.1.nk
-> Setnk(2) with fnk[2]=/home/marco/Workspace/vetr/bk071.2.nk

kSEMAWc - Marco Montecchi

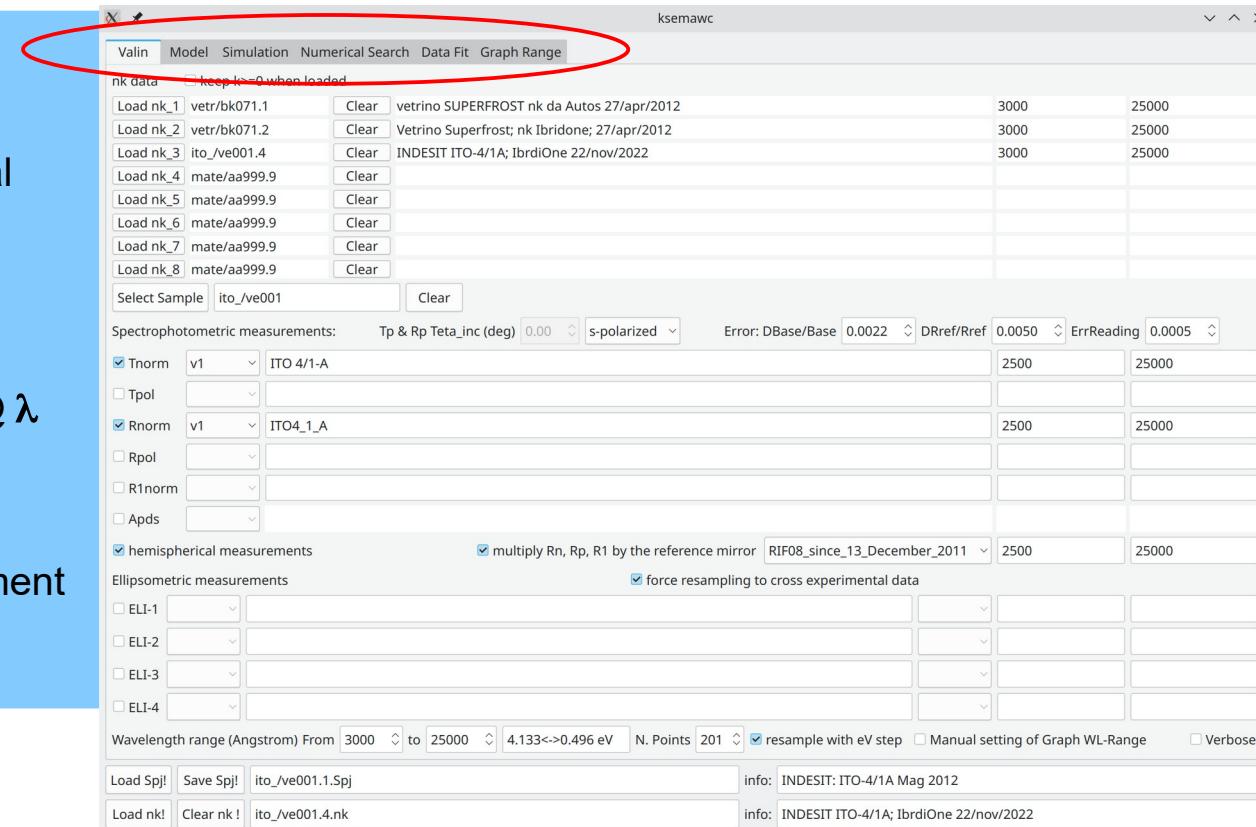
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Part III : initial GUI -Valin tab

GUI organized in 6 tabs

ordered according to the workflow:

- 1) **Valin:** load known *nk*-files and experimental spectra, re-sampled on 201 points (default)
- 2) **Model:** set the model of the optical device
- 3) **Simulation:** set and draw simulations
- 4) **Numerical Search:** search in **n-k space @ λ** or exhaustive solution search in $\lambda-n$ space
- 5) **Data Fit:** standard best fit or IbridOne
- 6) **Graph range:** plot and GUI graphic management



Part III : Model tab

Layered model (max 9 layers)

Type of layer:

1) bulk = thick = incoherent interfaces

2) homo. film = thin film

3) inhom. film = graded-index thin film

Materials (up to 8):
are set in Material#J
(#1 is the unknown !)

Then, “material” has to be assigned for each layer

ksemawc

Valin Model Simulation Numerical Search Data Fit Graph Range

Model of the optical device (from Front to Back)

type	Move	d(mm-A)	rough (A)	GRAD-n	dGRAD-n/dE	CURV-n	GRAD-k	CURV-k	material
inhomo. film	-	dw	2508.65	0.0	0.0209	0.000	-0.0076	0.0000	Material #1
bulk	up	dw	1.00	0.0	0.0000	0.000	0.0000	0.0000	Material #2
bulk	up	dw	0.00	0.0	0.0000	0.000	0.0000	0.0000	Material #1
bulk	up	dw	0.00	0.0	0.0000	0.000	0.0000	0.0000	Material #1
bulk	up	dw	0.00	0.0	0.0000	0.000	0.0000	0.0000	Material #1
bulk	up	dw	0.00	0.0	0.0000	0.000	0.0000	0.0000	Material #1
bulk	up	dw	0.00	0.0	0.0000	0.000	0.0000	0.0000	Material #1
bulk	up	dw	0.00	0.0	0.0000	0.000	0.0000	0.0000	Material #1
bulk	up	-	0.00	0.0	0.0000	0.000	0.0000	0.0000	Material #1

N. layers 2 Symmetric on 2nd face inhomogeneity as 23 subfilm computing <f(x)> with N= 3

Materials

Material #1	unknown	n	k	with	EMA	f
Material #2	vetr/bk071.2	1	0	<input type="checkbox"/>	air n=1 k=0	0.000
Material #3	constant nk	1	0	<input type="checkbox"/>	air n=1 k=0	0.000
Material #4	constant nk	1	0	<input type="checkbox"/>	air n=1 k=0	0.000
Material #5	constant nk	1	0	<input type="checkbox"/>	air n=1 k=0	0.000
Material #6	constant nk	1	0	<input type="checkbox"/>	air n=1 k=0	0.000
Material #7	constant nk	1	0	<input type="checkbox"/>	air n=1 k=0	0.000
Material #8	constant nk	1	0	<input type="checkbox"/>	air n=1 k=0	0.000
output SF	constant nk	1	0	<input type="checkbox"/>	air n=1 k=0	0.000
input SF	constant nk	1	0	<input type="checkbox"/>	air n=1 k=0	0.000
input PDS	constant nk	1	0	<input type="checkbox"/>	air n=1 k=0	0.000
input ELI-1	constant nk	1	0	<input type="checkbox"/>	air n=1 k=0	0.000
input ELI-2	constant nk	1	0	<input type="checkbox"/>	air n=1 k=0	0.000
input ELI-3	constant nk	1	0	<input type="checkbox"/>	air n=1 k=0	0.000
input ELI-4	constant nk	1	0	<input type="checkbox"/>	air n=1 k=0	0.000

ito_ /ve001.1.Spj info: INDESIT: ITO-4/1A Mag 2012
 ito_ /ve001.4.nk info: INDESIT ITO-4/1A; IbrdiOne 22/nov/2022

Part III : Simulation tab

To compare simulated with experimental

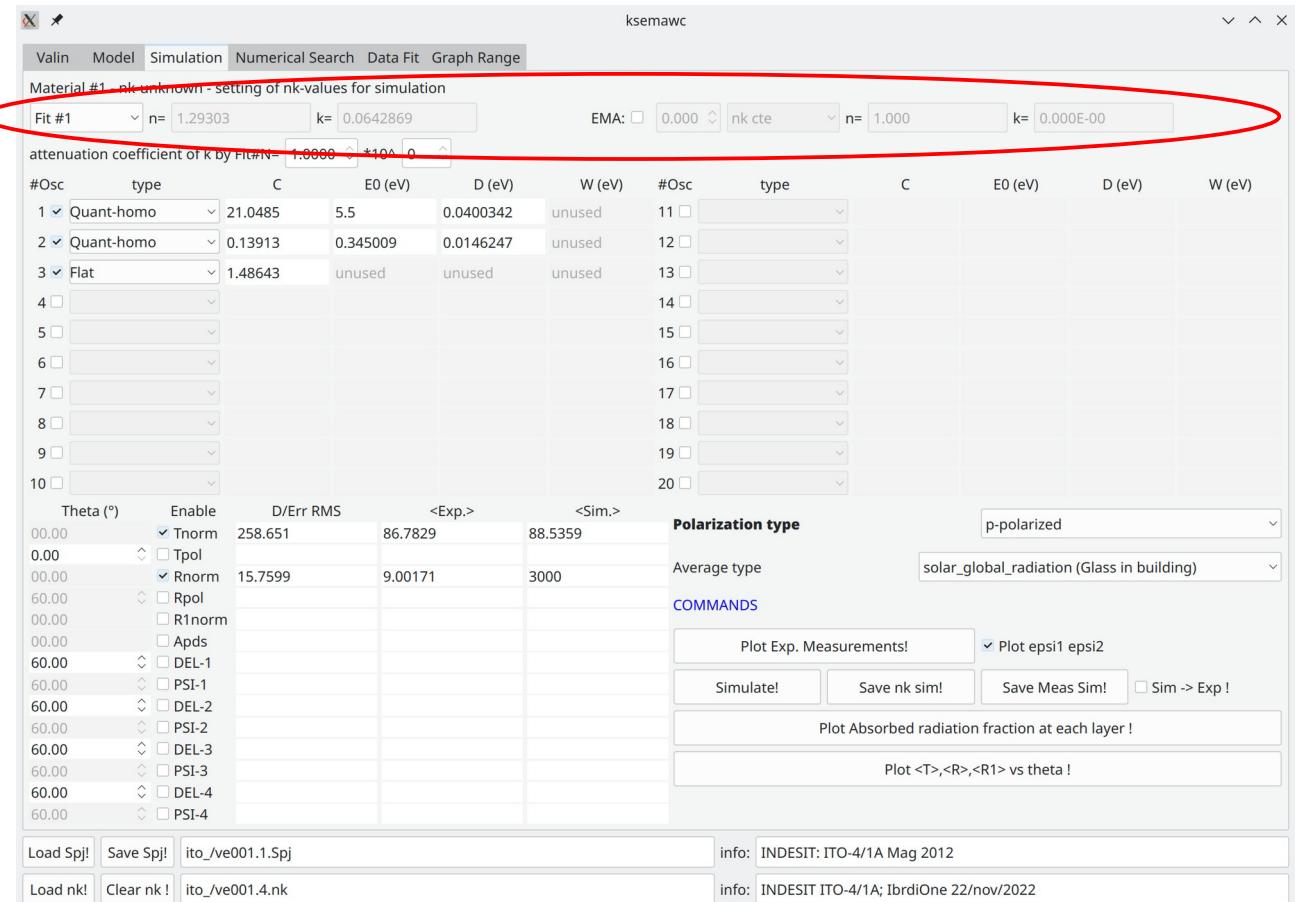
nk-unknown has to be set among:

- Constant nk
- Fit #M $1 \leq M \leq 7$
- Nk-file #M $1 \leq M \leq 8$
- Nk-DataFit from the last computation

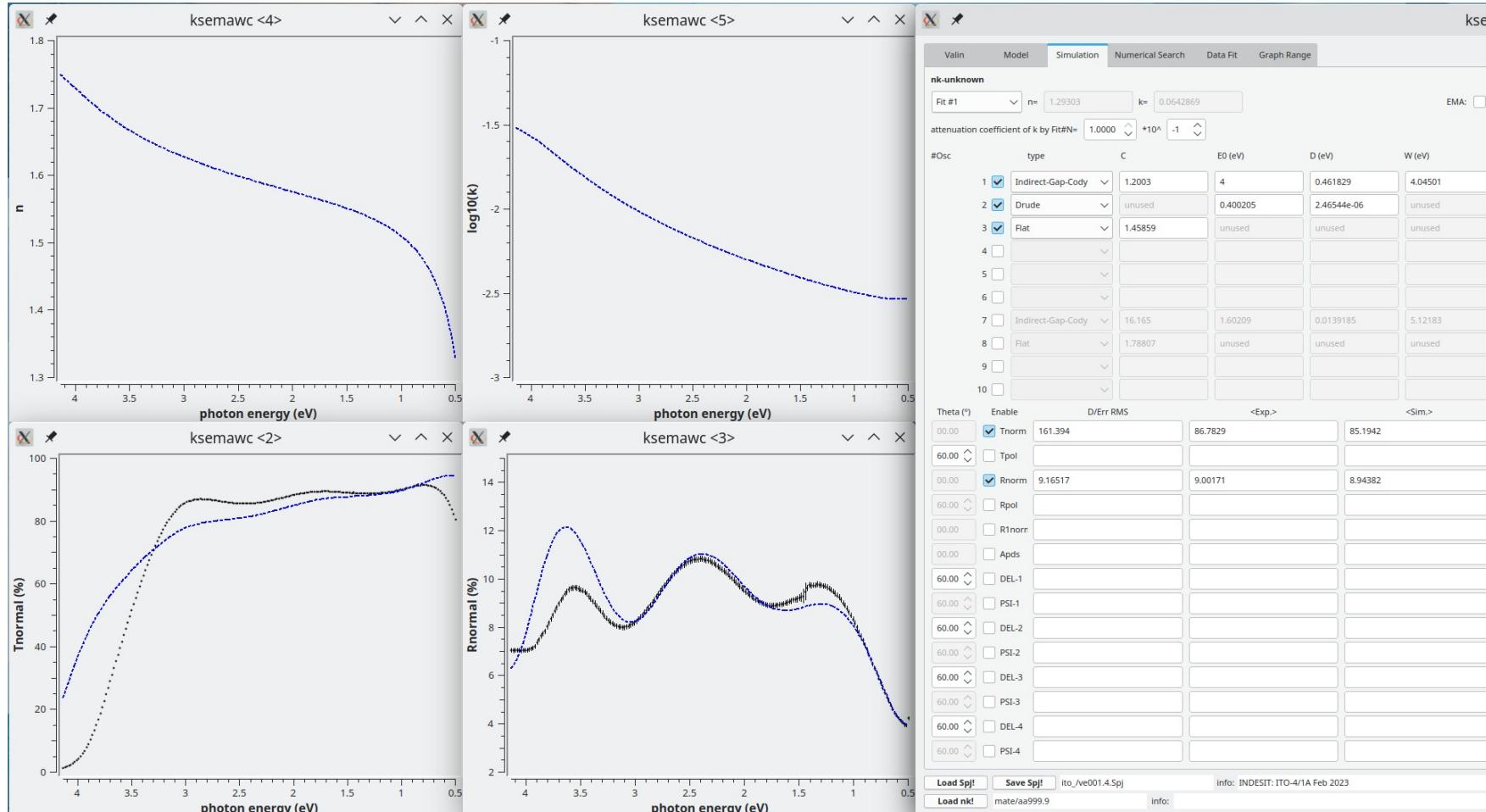
Two different materials can be combined according to the Effective Medium Approximation

Available actions:

- 1) Plot **experimental** spectra
- 2) Plot **simulated** spectra
- 3) Set the weights for computing mean values
- 4) Plot mean values versus incidence angle
- 5) Plot Absorptance at each layer



Part III : Simulation tab

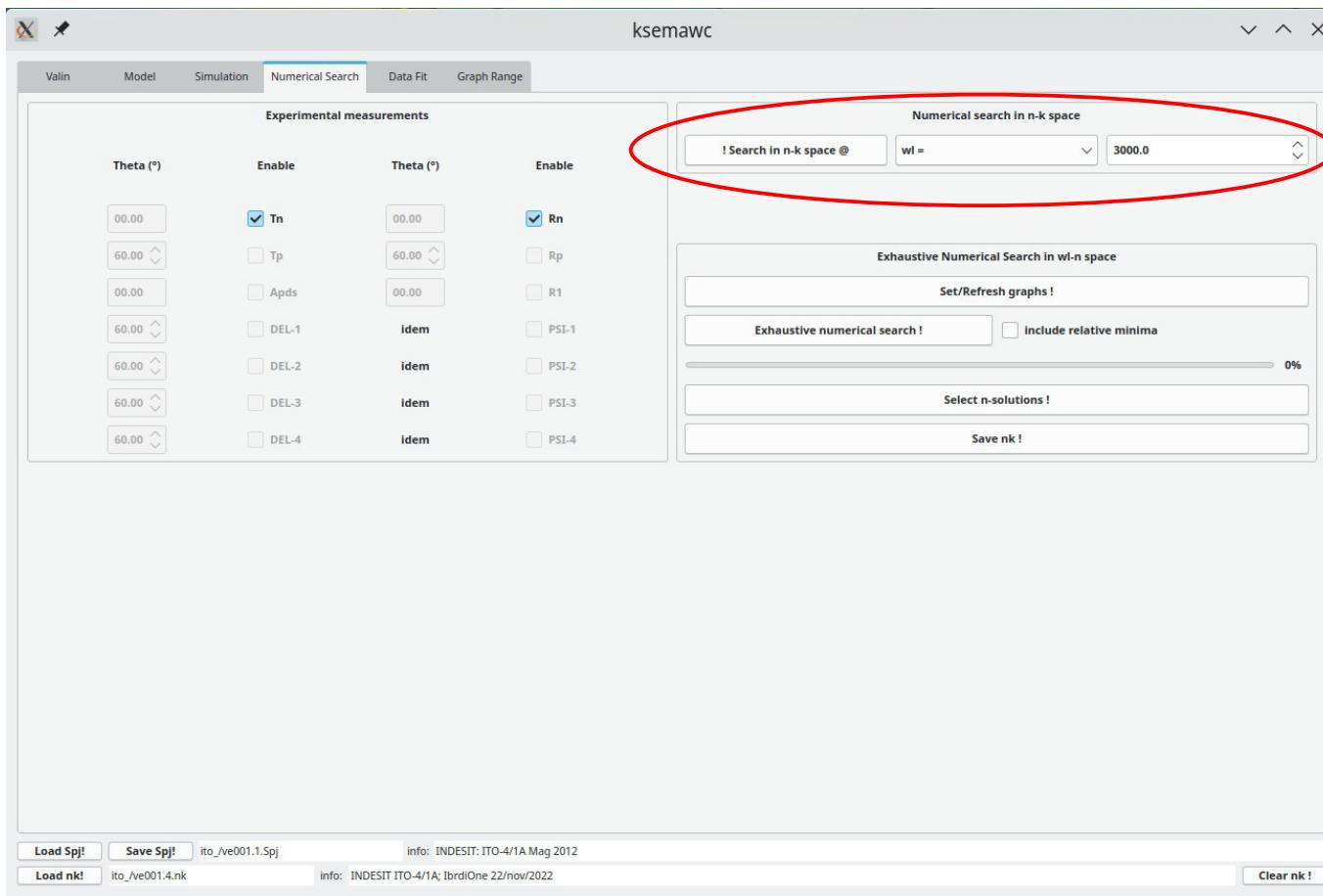
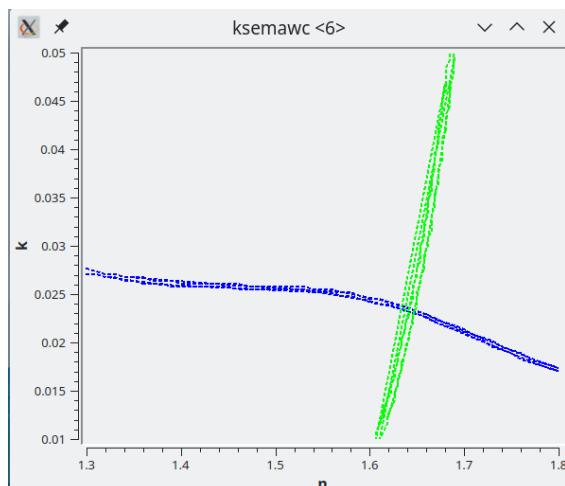


Part III : Numerical Search

Numerical search of solution $n-k$

Available methods:

- 1) Search in n-k space @ λ



The screenshot shows the "Numerical Search" tab of the ksemawc software. The interface includes several sections:

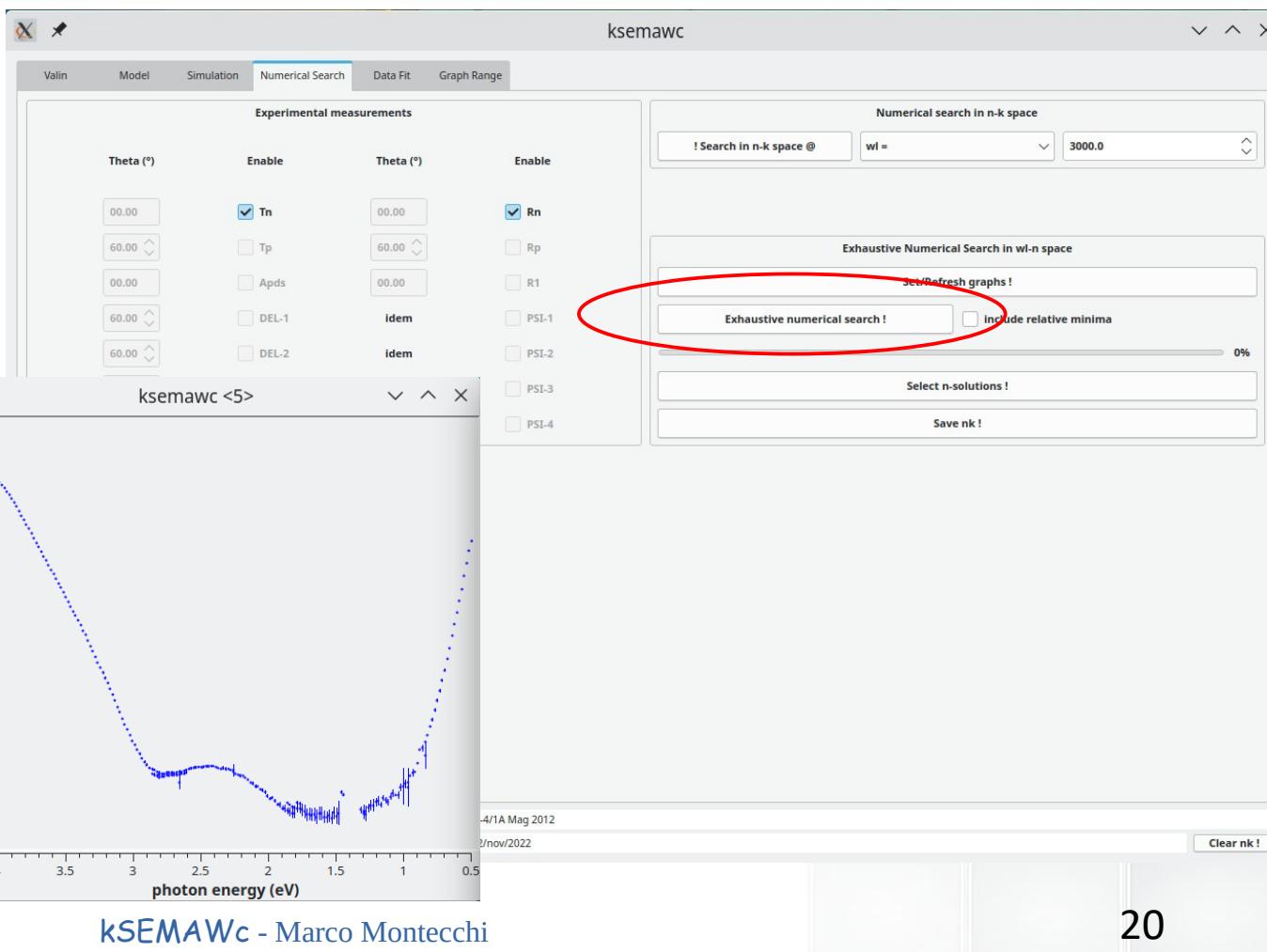
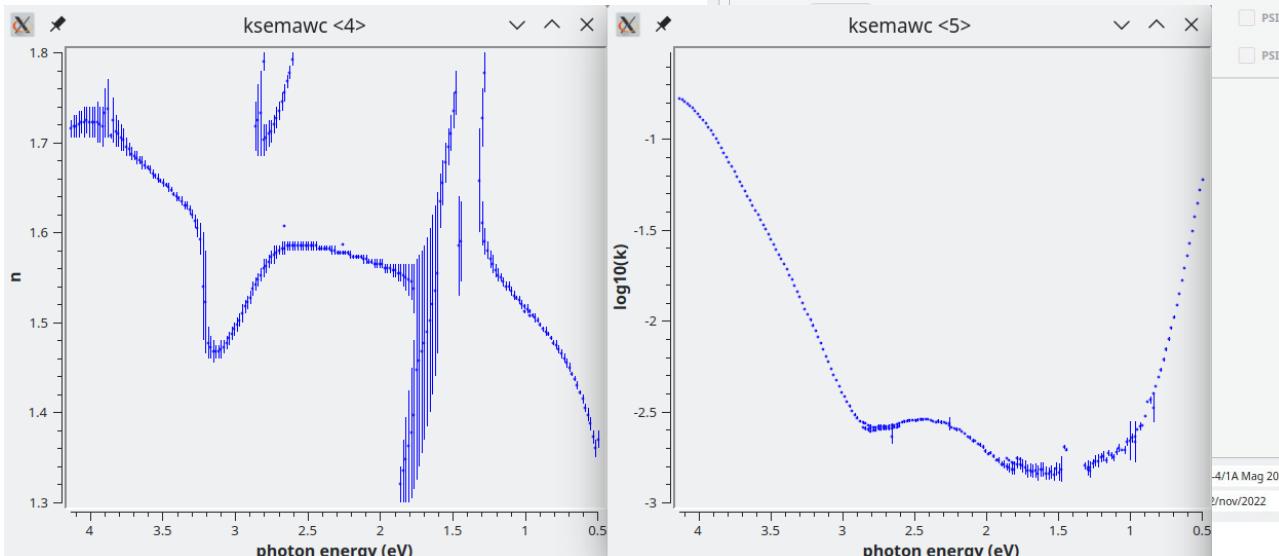
- Experimental measurements:** A grid of checkboxes for various parameters (Tn, Rp, etc.) with dropdown menus for angles.
- Numerical search in n-k space:** A section with a red circle highlighting the search parameters:
 - Search in n-k space @ λ
 - wl = 3000.0
- Exhaustive Numerical Search in wl-n space:** Buttons for "Set/Refresh graphs!", "Exhaustive numerical search!", "include relative minima", "Select n-solutions!", and "Save nk!".
- File and Info:** Buttons for "Load Spj!", "Save Spj!", "Load nk!", and "Clear nk!". Status information at the bottom includes "info: INDESIT: ITO-4/1A Mag 2012" and "info: INDESIT ITO-4/1A; lbrdiOne 22/nov/2022".

Part III : Numerical Search

Numerical search of solution $n-k$

Available methods:

- 1) Search in n - k space @ λ
- 2) Exhaustive numerical search in λ - n space



Part III : Data Fit tab

Available actions:

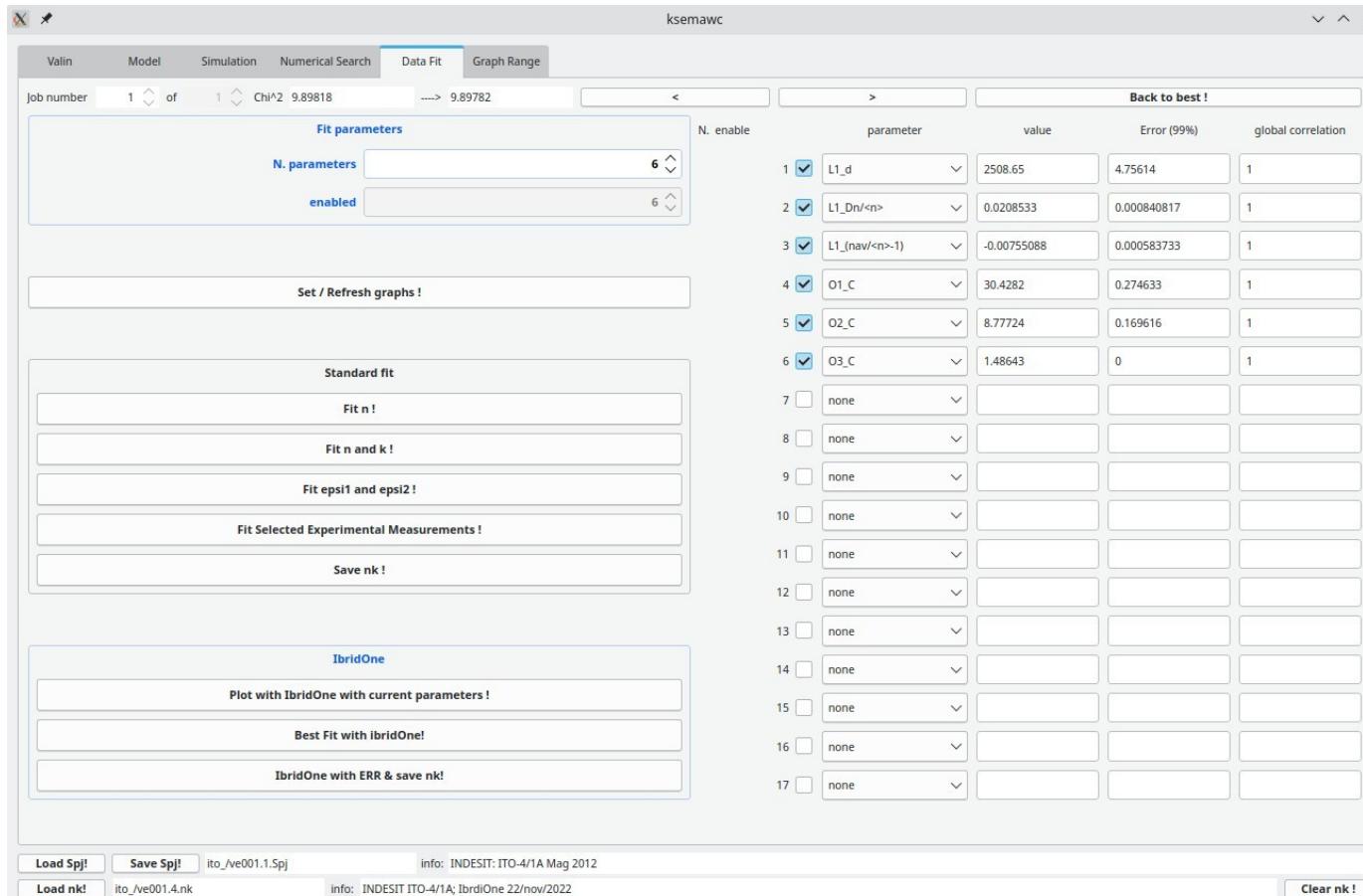
- 1) Fit of n data
- 2) Fit of n and k data
- 3) Fit of ε_1 and ε_2 data
- 4) Fit of experimental spectra
- 5) **IbridOne:**

Step-1: fit $R(\lambda)$ with

$$n = n(\lambda, p_1, p_2, \dots, p_M)$$

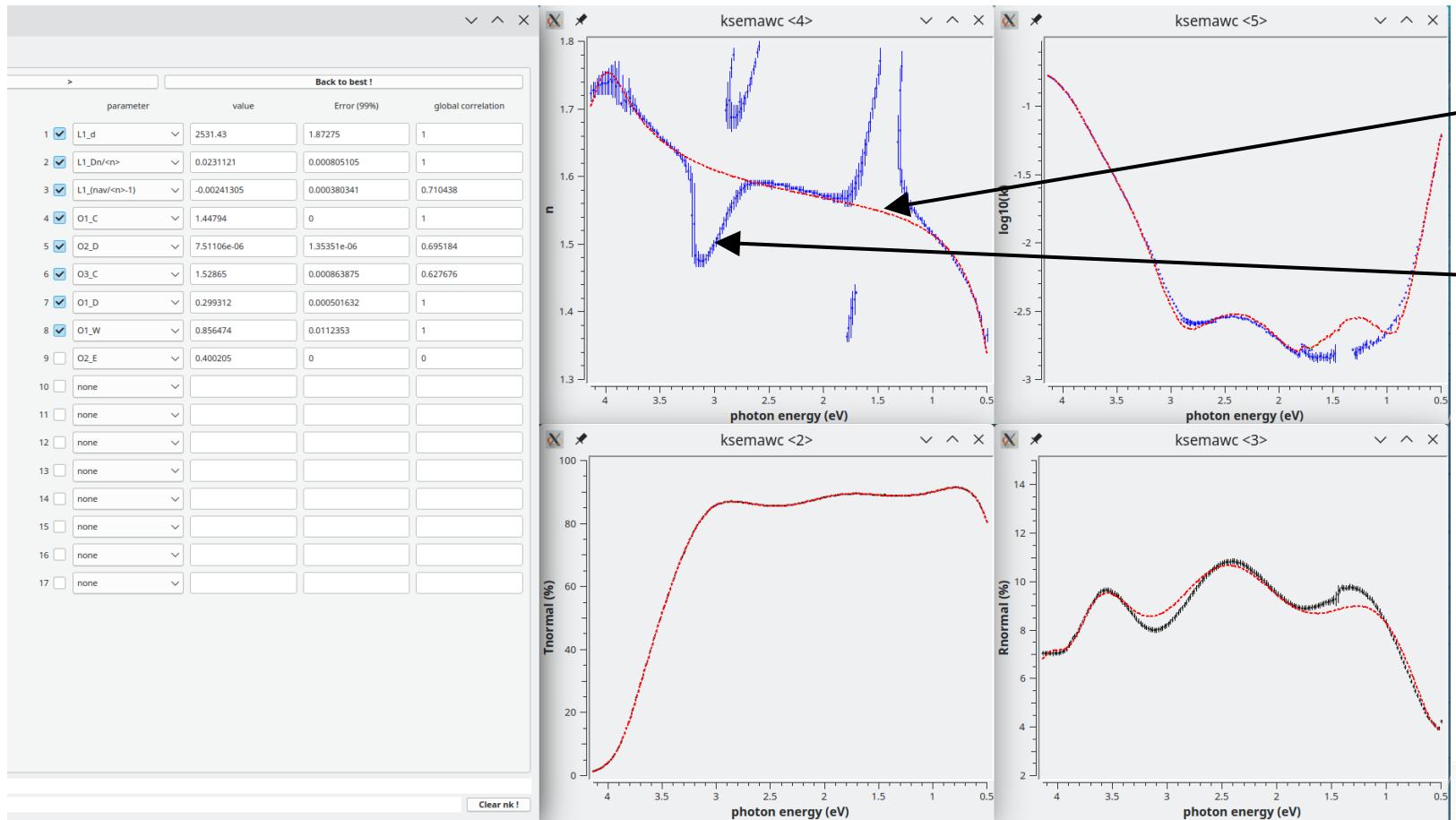
Step-2: compute $k(\lambda)$ from $T(\lambda)$ given $n(\lambda)$

Called by Levenberg-Marquardt



	N. enable	parameter	value	Error (99%)	global correlation
1	<input checked="" type="checkbox"/>	L1_d	2508.65	4.75614	1
2	<input checked="" type="checkbox"/>	L1_Dn/<n>	0.0208533	0.000840817	1
3	<input checked="" type="checkbox"/>	L1_nav/<n>-1	-0.00755088	0.000583733	1
4	<input checked="" type="checkbox"/>	O1_C	30.4282	0.274633	1
5	<input checked="" type="checkbox"/>	O2_C	8.77724	0.169616	1
6	<input checked="" type="checkbox"/>	O3_C	1.48643	0	1
7	<input type="checkbox"/>	none			
8	<input type="checkbox"/>	none			
9	<input type="checkbox"/>	none			
10	<input type="checkbox"/>	none			
11	<input type="checkbox"/>	none			
12	<input type="checkbox"/>	none			
13	<input type="checkbox"/>	none			
14	<input type="checkbox"/>	none			
15	<input type="checkbox"/>	none			
16	<input type="checkbox"/>	none			
17	<input type="checkbox"/>	none			

Part III : Data Fit tab



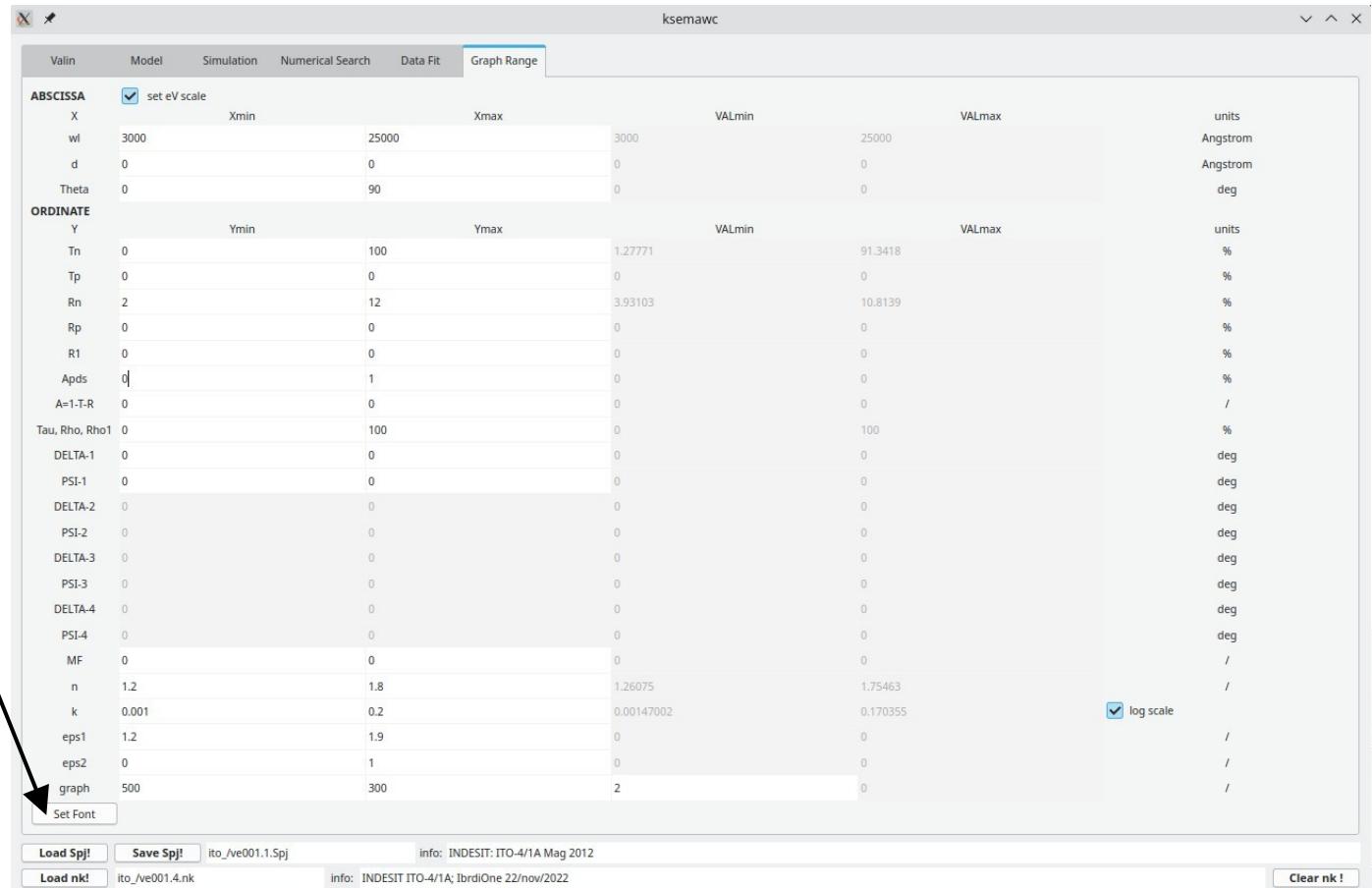
IbridOne (red)

Exhaustive
Numerical
Search (blue)

Part III : Graph Range tab

Option management of

- Plots (X-Y range,
Energy/Wavelength abscissa,
log scale for k)
- GUI (font type and size)



How can you help?

BETA-TESTER:

- 1) Testing kSEMAWc and reporting bugs
- 2) Proposing improvements to make GUI and usage clearer
- 3) Asking for new features (of general relevance)
- 4) ...

Anyone interested in participating at any level is welcome!

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- 4) ...

Computer experts:

- Testing installation from source
- Improving the code structure
- ...

Anyone interested in participating at any level is welcome!

Contributors

Alberto Mittiga, for his factual collaboration in improving optical constant models about electronic transitions in materials with continuous state density, in the Windows porting as well as in the drafting of the manual

Enrico Nichelatti, for the wise search for analytical solutions of the integrals on the density of the states, as well as for the transfer in LaTex of this manual

Claudia Malerba and Francesca Menchini, for their constant goad to test and improve kSEMAWc to characterize semiconductor materials

Francesco Biccari, for his useful suggestions for simplifying the software distribution

Luca Serenelli, for his support in outlining the Linux installation procedure

What's next?

Alberto Mittiga, will present an overview of the oscillators used for modeling the dielectric constant

You can ask for further webinars on specific topics, for instance

- Substrate characterization
- Dielectric thin film characterization
- Semiconductor thin film characterization
-

