Optical Parameters from Transmittance Spectrum (OPTIFIT)

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OPTIFIT FEATURES

OPTIFIT analyzes the optical transmittance of thin films in the UV-visible range and performs a parametric fit to a well-known formula (see the *Fitting Function* section), allowing the calculation of the refractive index and the extinction coefficient of the film as a function of the wavelength. Outstanding features of the software include a graphical interface that allows wavelength range selection for the fit, and the incorporation of an automated procedure for the approximated estimation of the refractive index and thickness of the film.

FITTING FUNCTION

The mathematical dependence between the transmittance spectrum and the optical parameters have been taken from Swanepoel [R Swanepoel, J. Phys. E: Sci. Instrum. 16 (1983) 1214]. The Sellmeier dispersion relation has been used for the refractive index [B. Tatian, Appl. Opt. 23 (1984) 4477], while the expression for the extinction coefficient includes an absorption band gap zone [N. Ghobadi, Int. Nano Lett. 3 (2013) 2] and a Taylor expansion on the frequency as a dispersion relation. The effect of the roughness has been included using the approach by Tikhonravov et. al [A.V. Tikhonravov, M.K. Trubetskov, A.A. Tikhonravov, A. Duparre, Appl. Opt. 42 (2003) 5140]. Finally, the estimation of the thickness and refractive index is taken from the review by Poelman and Smet [D. Poelman and P.F. Smet, J. Phys. D: Appl. Phys. 36 (2003) 1850].

COMPUTER REQUIREMENTS

OPTIFIT requires a computer that may run MATLAB 2014a. OPTIFIT has been compiled with a 64 bit compiler for windows.

DISTRIBUTION

The software OPTIFIT is freely distributable and can be downloaded from the webpage http://nanoscops.icmse.csic.es. When referring to it, cite the manuscript appearing in the *Reference* section.

INSTALLATION

Native language of OPTIFIT is MATLAB. It is therefore necessary to have installed the freely distributable MATLAB Compiler Runtime (MCR) application, which can be downloaded from the webpage of MATHWORKS:

http://www.mathworks.com/supportfiles/downloads/R2014a/deployment_files/R2014a/installers/win64/MCR_R2014a_win64_installer.exe

Once the MCR is installed, open OPTIFIT.exe to start the program. Please, take into account that the first time it is executed, it may take some time to start due to the initialization of the MCR.

RUNNING OPTIFIT

Double click on OPTIFIT.exe and wait a few seconds until the MCR executes and the graphic interface of OPTIFIT opens.

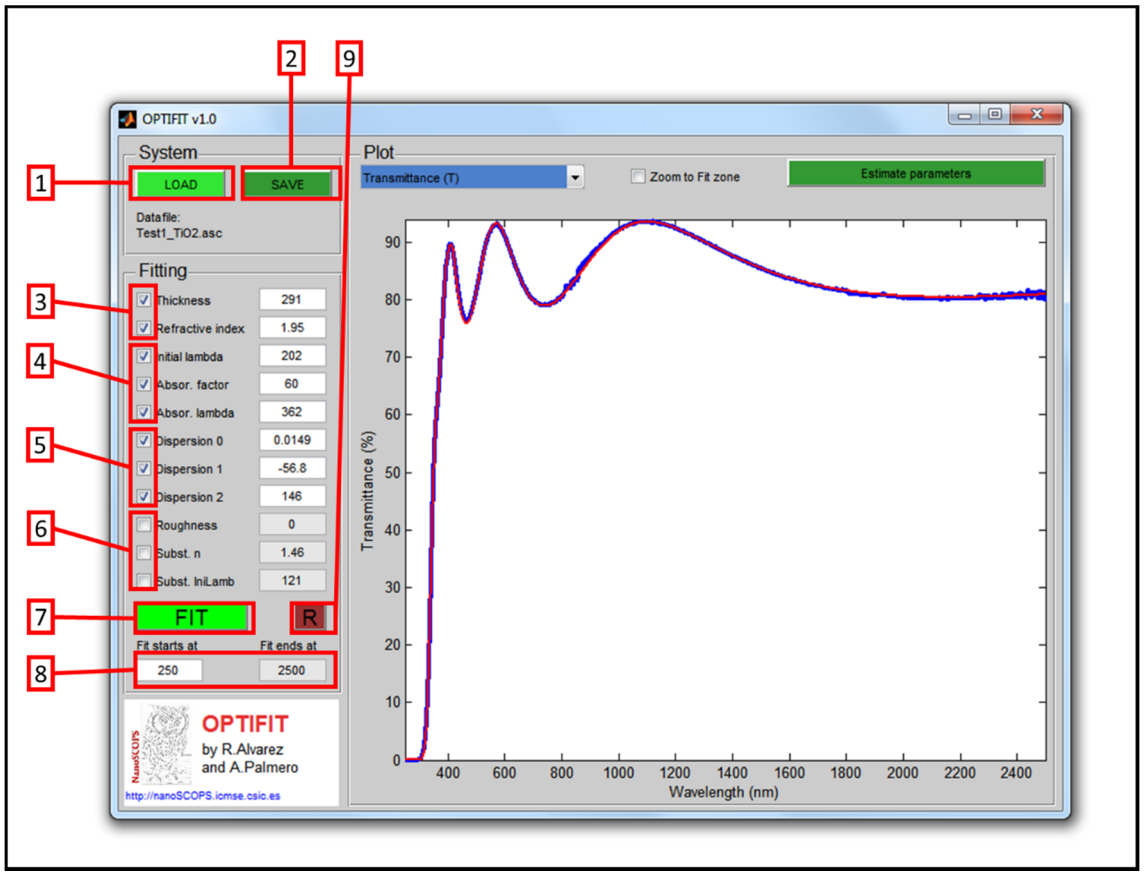
USING OPTIFIT

SYSTEM:

- LOAD (1): OPTIFIT accepts ASCII data formatted in two columns: wavelength (nm) and transmittance (%). For detailed formatting specs please examine with a text editor the Test files supplied within the "Examples" folder.

- SAVE (2): Three files will be created in the same folder of the selected data. If the name of the datafile was "FileName.dat", the files would be:
    - "FileName_Data.dat": An ASCII file with 5 columns: Wavelength (in nm), Experimental Transmittance (%), Transmittance Fit (%), Refractive Index, and Extinction Coefficient.
    - "FileName_FitParam.dat": An ASCII file with the values of the fitting parameters.
    - "FileName_Graph.png": A PNG graph file with a screenshot of the program at the moment of the save. This file is for logging and identification of fitting conditions only, so the resolution is low. A good quality graph should be obtained by plotting the datasets.

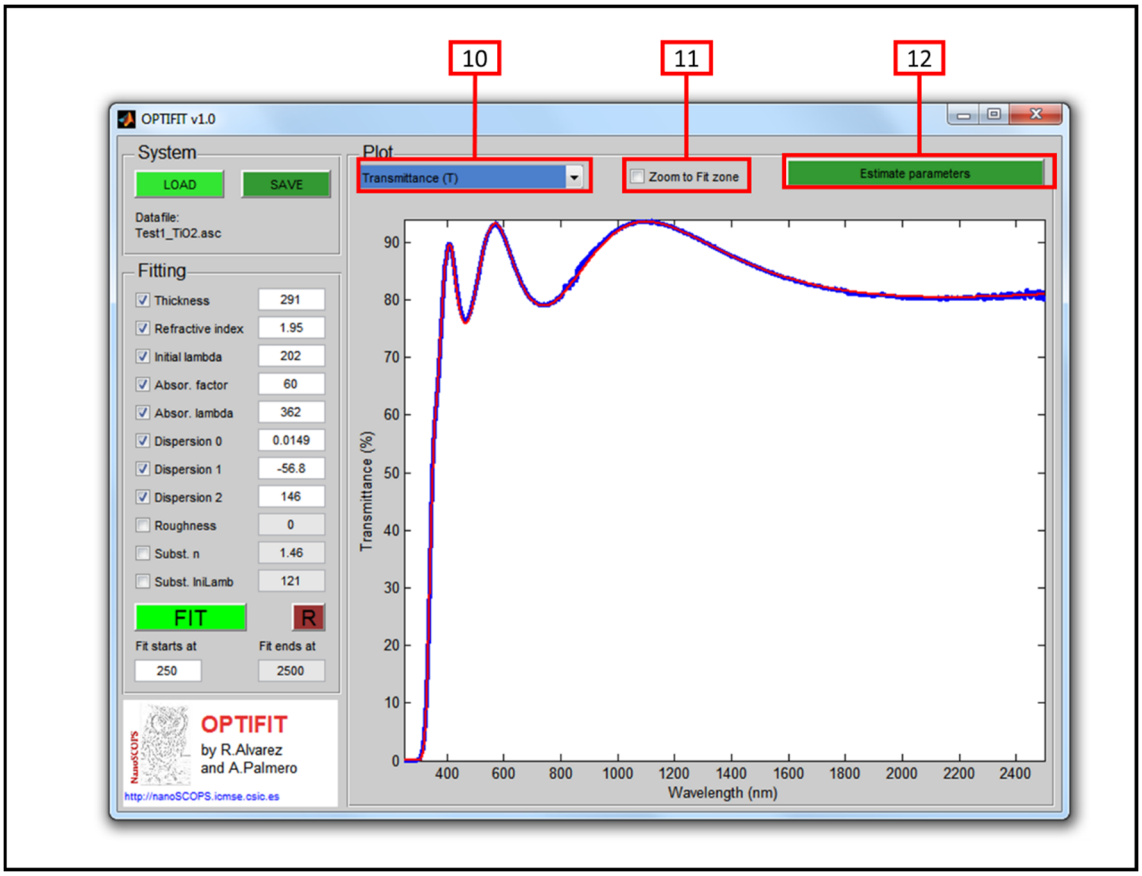
  If subsequent fits are performed on the same dataset, files with an added number after "Filename" will be created, so the results of previous fits are not deleted.



FITTING:

- Thickness (3a): Thickness of the thin film in nm. As a rule of thumb, this parameter will increase the number of interference oscillations in the transmittance.
- Refractive index (3b): Value of the refractive index at 589.29 nm (standard definition). As a rule of thumb, this parameter will increase the amplitude of the interference oscillations in the transmittance.
- Initial lambda (4a): Starting wavelength (nm) for the transmittance fit.
- Absorption factor (4b): Factor for the absorption component of the extinction coefficient.
- Absorption lambda (4c): Wavelength (nm) from which the absorption component of the extinction coefficient can be neglected.
- Dispersion 0 (5a), Dispersion 1 (5b) and Dispersion 2 (5c): Coefficients of the dispersion component of the extinction coefficient.
- Roughness (6a): Roughness of the thin film (nm).
- Substrate n (6b): Value of the refractive index of the substrate at 589.29 nm (standard definition). The default value is that of SiO_2.
- lamb0_subs (6c): Starting wavelength (nm) for the refractive index of the substrate. The default value is that of SiO_2.

- FIT (7): Starts fitting procedure, taking as free parameters those that are selected.
- Fitting Range (8): allows selection of lower and upper bounds in wavelength (in nm) for the fit.
- Reset fitting parameters (9): All parameters reset to their default values.



PLOT: OPTIFIT provides a graphical interface where both the experimental transmittance data (in blue) and the numerical fit (in red) are plotted. Clicking with the mouse on a data plot generates an information box with the numerical coordinates of the selected datapoint.

- Select result to show (10): The user can choose to represent either the transmittance and the corresponding fit, or the calculated values for the refractive index and the extinction coefficient versus the wavelength.
- Zoom to Fit Zone (11): If the fitting range (8) has been reduced to a smaller interval, by checking this box the experimental data plotted will also be restricted to the selected zone, providing a more detailed view of the fit.
- Estimate parameters (12): This button activates the automatic estimation of the parameters Thickness (3a) and Refractive Index (3b). In order to do so, OPTIFIT will ask the user to click at two consecutive interference maxima and then at the minimum between them. The accuracy of this estimation depends on several factors, such as the number of interference maxima or the dispersion of the film, but it can provide a starting point for the iterative fitting procedure.

RECOMMENDED FITTING PROTOCOL

Fitting a dataset with a non-lineal equation that incorporates 11 parameters can certainly be quite a challenge, requiring both patience and an understanding of the physical meaning behind those parameters. In general, there will not be a systematic procedure that provides a good fit for any possible dataset. A sensible protocol to perform the fit is:

1) Estimate parameters 3 using the automatic estimation (12).
2) Allow variation of parameters 3 and use FIT (7).
3) Allow variation of parameters 4 and use FIT (7).
4) Allow variation of parameters 5 and use FIT (7).

Sometimes is better to exchange steps 2 and 3, if step 2 makes the fit worse.

As a final recommendation, if the fit does not work in the whole wavelength range, try fitting in a smaller range, get the parameters right, and extend the range after.

UPDATES

Click the icon with the owl at the bottom of the OPTIFIT panel to access the webpage of NanoSCOPS and check for updates.

REFERENCE

R. Alvarez, A. Garcia-Valenzuela, C. Lopez-Santos, F.J. Ferrer, V. Rico, E. Guillen, M. Alcon-Camas, R. Escobar-Galindo, A.R. Gonzalez-Elipe, A. Palmero, “High Rate Deposition of Stoichiometric Compounds by Reactive Magnetron Sputtering at Oblique Angles”, accepted for publication in Plasma Processes and Polymers (2016).