Estimation of the thickness and the optical parameters of several superimposed thin films using optimization

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April 17, 2007

Abstract

The Reverse Engineering problem addressed in the present research consists in estimating the thicknesses and the optical parameters of several thin films deposited in a transparent substrate using transmission data through the whole stack. The same methodology can be used if the available data correspond to reflectance. The case of a single film has been addressed in previous works. Complete freely available software may be found in the PUMA project webpage *http://www.ime.usp.br/∼egbirgin/puma/*.

Keywords: Optical constants, thin films, optimization, numerical algorithms, Reverse Engineering.

1 Introduction

Reverse Engineering is the process of discovering the structure of a system by means of the analysis of its behavior. From the mathematical point of view, Reverse Engineering uses

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to be an Inverse Problem, in the sense that the available data for recovering the structure is usually incomplete or noisy and, so, infinitely many unstable or physically meaningless solutions are expected.

Here we have a system composed by a stack of thin films deposited on a transparent substrate. We aim to discover the structure of the system using transmittance data. The structure of the system is represented by the thickness, the absorption coefficient function and the refractive index function of each film.

The films can be deposited on one or both sides of a transparent substrate.

NOTA 1 (IVAN): Acá el comandante escribe la importancia física de esto y comentarios bibliograficos.

This paper is organized as follows. The mathematical model of the estimation problem is presented in Section 2. The optimization technique is described in Section 3. Section 4 presents the numerical experiments. Conclusions are stated in Section 5.

2 Mathematical model of the estimation problem

The physical object that we have in mind is a stack of thin films deposited on both sides of a transparent substrate. As usually, we define the *top* of the stack as the side where light is incident. Of course, the *bottom* is the opposite side. Measurements of transmittance are taken using a pendorchómetro de absorcin ictícola. (Reflectance measurements can also be used emplying the methodology of this paper.) These measurements are available for a wavelength range of $\lambda_{\min}$ to $\lambda_{\max}$ nanometers.

The refractive index s of the substrate is known. The thickness of the substrate is also known but it plays no role in the calculations. The reason for this is that the substrate is transparent and its thickness is much larger than the thicknesses of the films.

For each deposited film we have, as unknown quantities, the thickness, the refractive index (as a function of the wavelength) and the attenuation coefficient (as a function of the wavelength too [6, 12]).

Assume that $m_t \geq 0$ films are deposited on the top of the substrate and $m_b \geq 0$ films are deposited on the bottom. For all $i = 1, \ldots, m_t$, $\lambda \in [\lambda_{\min}, \lambda_{\max}]$ we denote:

$$d_i^t = \text{ thickness of top film } i,$$

$$n_i^t(\lambda) = \text{ refractive index of top film } i,$$

$$\kappa_i^t(\lambda) = \text{ attenuation coefficient of top film } i.$$

Analogously, for all $i = 1, \ldots, m_b$ we denote:

$$d_i^b = \text{ thickness of bottom film } i,$$

$$n_i^b(\lambda) = \text{ refractive index of bottom film } i,$$

$$\kappa_i^b(\lambda) = \text{ attenuation coefficient of bottom film } i.$$

For each wavelength λ, the theoretical transmittance and the theoretical reflectance are functions of thicknesses, refractive indices and attenuation coefficients, so:

$$T^{\text{theoretical}}(\lambda) = T(s(\lambda), \{d_i^t\}_{i=1}^{m_t}, \{n_i^t(\lambda)\}_{i=1}^{m_t}, \{\kappa_i^t(\lambda)\}_{i=1}^{m_t}, \{d_i^b\}_{i=1}^{m_b}, \{n_i^b(\lambda)\}_{i=1}^{m_b}, \{\kappa_i^b(\lambda)\}_{i=1}^{m_b}). \tag{1}$$

In order to simplify the notation, we write:

$$\begin{aligned} d_{\text{top}} &= \{d_i^t\}_{i=1}^{m_t}, & d_{\text{bottom}} &= \{d_i^b\}_{i=1}^{m_b}, \\ n_{\text{top}}(\lambda) &= \{n_i^t(\lambda)\}_{i=1}^{m_t}, & n_{\text{bottom}}(\lambda) &= \{n_i^b(\lambda)\}_{i=1}^{m_b}, \\ \kappa_{\text{top}}(\lambda) &= \{\kappa_i^t(\lambda)\}_{i=1}^{m_t}, & \kappa_{\text{bottom}}(\lambda) &= \{\kappa_i^b(\lambda)\}_{i=1}^{m_b}. \end{aligned}$$

and

$$d_{\text{all}} = \{d_{\text{top}}, d_{\text{bottom}}\}, \quad n_{\text{all}} = \{n_{\text{top}}, n_{\text{bottom}}\}, \quad \kappa_{\text{all}} = \{\kappa_{\text{top}}, \kappa_{\text{bottom}}\}$$

So, (1) can be written as:

$$T^{\text{theoretical}}(\lambda) = T\left(s(\lambda), d_{\text{all}}, n_{\text{all}}(\lambda), \kappa_{\text{all}}(\lambda)\right).$$

When $m_t = 1$ and $m_b = 0$, the formula (1) can be the one given in [18] and used in [2, 3, 14] for recovering optimal parameters of a single film deposited on the top of a transparent substrate [15]. A general formula for arbitrary m_t and m_b is discussed in Sections 1.4–1.6 of [7]. Proofs that the integrals along substrate thickness correspond to the analytical expression showed in [7] can be found in [13]. In this work we use a formula introduced by Ventura [19] which, although equivalent to the ones given in [7] is better suited for numerical computations. In particular, derivatives of the parameters involved in (1) are easily available when we use these formulae.

Using the pendorchómetro, we obtain measurements $T^{\text{meas}}(\lambda_i)$ for wavelengths $\lambda_i, i = 1, \ldots, N$, where

$$\lambda_{\min} \leq \lambda_1 < \ldots < \lambda_N \leq \lambda_{\max}.$$

Ideally, for all $i = 1, \ldots, N$, the true parameters should satisfy the equations

$$T^{\text{meas}}(\lambda_i) = T\left(s(\lambda_i), d_{\text{all}}, n_{\text{all}}(\lambda_i), \kappa_{\text{all}}(\lambda_i)\right). \tag{2}$$

However, this is a system with $(m_t + m_b)(2N + 1)$ unknowns and only $2N$ equations, which, very likely, is highly underdetermined. Moreover, observations are subject to measurement errors and, last but not least, the model is not completely adequate to reality, since assumptions like homogeneity, complete substrate transparency and parallelism of interfaces are hard to be satisfied exactly. The many degrees of freedom that are inherent to this problem lead us to introduce empirical and phenomenological constraints that must

be satisfied by the parameters of the films under consideration. See [2] and [20] for the application of this philosophy to the one-film estimation problem with transmission and reflectance data, respectively. Namely, instead of considering the nonlinear system (2) we define the optimization problem

$$\begin{array}{ll} \text{Minimize} & \sum_{i=1}^{M} \left[T(s(\lambda_i), d_{\text{all}}, n_{\text{all}}(\lambda_i), \kappa_{\text{all}}(\lambda_i)) - T^{\text{meas}}(\lambda_i)\right]^2 \\ \text{subject to} & \text{Physical Constraints.} \end{array} \tag{3}$$

In the one-film case this strategy has been successfully used many times under the PUMA project (see [21]).

We use the same constraints that are employed in the one-film case [2], which are quite suitable for amorphous a-semiconductor thin films in the neighborhood of the fundamental absorption edge of a-semiconductors. For completeness, these constraints are described below. We assume that $n(\lambda)$ is the refraction index and $\kappa(\lambda)$ is the attenuation coefficient of a generic film in the stack.

PC1: $n(\lambda) \geq 1$ and $\kappa(\lambda) \geq 0$ for all $\lambda \in [\lambda_{\text{min}}, \lambda_{\text{max}}]$;

PC2: $n(\lambda)$ and $\kappa(\lambda)$ are decreasing functions of λ;

PC3: $n(\lambda)$ is convex;

PC4: there exists $\lambda_{\text{infl}} \in [\lambda_{\text{min}}, \lambda_{\text{max}}]$ such that $\kappa(\lambda)$ is convex if $\lambda \geq \lambda_{\text{infl}}$ and concave if $\lambda < \lambda_{\text{infl}}$.

In [2] it has been showed that **PC1–PC4** will be satisfied if, and only if,

$$n(\lambda_{\text{max}}) \geq 1, \quad \kappa(\lambda_{\text{max}}) \geq 0, \tag{4}$$

$$n'(\lambda_{\text{max}}) \leq 0, \quad \kappa'(\lambda_{\text{max}}) \leq 0, \tag{5}$$

$$n''(\lambda) \geq 0 \text{ for all } \lambda \in [\lambda_{\text{min}}, \lambda_{\text{max}}], \tag{6}$$

$$\kappa''(\lambda) \geq 0 \text{ for all } \lambda \in [\lambda_{\text{infl}}, \lambda_{\text{max}}], \tag{7}$$

$$\kappa''(\lambda) \leq 0 \text{ for all } \lambda \in [\lambda_{\text{min}}, \lambda_{\text{infl}}], \text{ and} \tag{8}$$

$$\kappa'(\lambda_{\text{min}}) \leq 0. \tag{9}$$

As in [2], we eliminate the constraints of the problem, by means of a suitable change of variables. So, we write

$$n(\lambda_{\text{max}}) = 1 + u^2, \quad \kappa(\lambda_{\text{max}}) = v^2, \tag{10}$$

$$n'(\lambda_{\text{max}}) = -u_1^2, \quad \kappa'(\lambda_{\text{max}}) = -v_1^2, \tag{11}$$

$$n''(\lambda) = w(\lambda)^2 \text{ for all } \lambda \in [\lambda_{\min}, \lambda_{\max}], \tag{12}$$

$$\kappa''(\lambda) = z(\lambda)^2 \text{ for all } \lambda \in [\lambda_{\text{infl}}, \lambda_{\max}], \text{ and} \tag{13}$$

$$\kappa''(\lambda) = -z(\lambda)^2 \text{ for all } \lambda \in [\lambda_{\min}, \lambda_{\text{infl}}]. \tag{14}$$

Discretizing the equations above, we get:

$$h = (\lambda_{\max} - \lambda_{\min})/(N-1), \text{ and}$$

$$\lambda_i = \lambda_{\min} + (i-1)h \text{ for } i = 1, \ldots, N.$$

The measured transmittance at λ_i will be called T_i^{meas}. We will use the notation n_i, κ_i, w_i, and z_i for the estimates of $n(\lambda_i)$, $\kappa(\lambda_i)$, $w(\lambda_i)$, and $z(\lambda_i)$, for all $i = 1, \ldots, N$. The discretization of (10–14) gives:

$$n_N = 1 + u^2, \quad v_N = v^2, \tag{15}$$

$$n_{N-1} = n_N + u_1^2 h, \quad \kappa_{N-1} = \kappa_N + v_1^2 h, \tag{16}$$

$$n_i = w_i^2 h^2 + 2n_{i+1} - n_{i+2} \text{ for } i = 1, \ldots, N-2, \tag{17}$$

$$\kappa_i = z_i^2 h^2 + 2\kappa_{i+1} - \kappa_{i+2}, \quad \text{if } \lambda_{i+1} \geq \lambda_{\text{infl}}, \text{ and} \tag{18}$$

$$\kappa_i = -z_i^2 h^2 + 2\kappa_{i+1} - \kappa_{i+2}, \quad \text{if } \lambda_{i+1} < \lambda_{\text{infl}}. \tag{19}$$

Let us stress that these constraints must be satisfied by the refraction indices and the attenuation coefficients of all the films.

3 Optimization technique

The problem (3) with the constraints defined by (15)-(19) is an optimization problemwith $(m_t + m_b)(2N+1)$ variables.

The constraints are represented by the nonnegativity of thicknesses and the fact that the inflection points λ_{infl} must be in the range $[\lambda_{\min}, \lambda_{\max}]$. The remaining variables are unconstrained and dimensionless. These are the main reasons to deal with them in a different way than we do with thicknesses and inflection points. Our strategy is to define, for each set of inflection points and each set of thicknesses a different continuous unconstrained optimization problem whose variables are the ones defined by the refraction indices and the attenuation coefficients. As in [2], the unconstrained problems will be solved using the spectral gradient method [17] (see [5] for a comparative study with the spectral conjugate gradient in the estimation of the thickness and the optical constants of thin films). The high-level procedure is defined in the following algorithm.

Algorithm 3.1

Step 1. Define a coarse grid with respect to the variables *thicknesses* and *inflection points*.

Step 2. For each point of the grid solve the problem (3),(15)-(19) where the variables *thicknesses* and *inflection points* are fixed. Obtain the set of thicknesses and the inflection points of the grid that, after solving the unconstrained optimization problems, give the smallest sum of squares.

Step 3. Define a new refined grid in a vicinity of the best thicknesses and best inflection points obtained at Step 2.

Step 4. Solve the unconstrained optimization problems defined by each point of the new grid. Adopt the solution that gives the smallest value of the sum of squares as the output of the algorithm.

For a system with two films, the initial coarse grid for the thickness is given by uniformly distributed points in the box $[d^1_{\min}, d^1_{\max}] \times [d^2_{\min}, d^2_{\max}]$, where $d^i_{\min}$ and $d^i_{\max}$ are (for film i) the lower and upper bound estimates of the film thicknesses, respectively. To estimate the inflection point we proceed in an analogous way: the initial coarse grid is given by uniformly distributed points in the box $[F^1_{\min}, F^1_{\max}] \times [F^2_{\min}, F^2_{\max}]$, where $F^i_{\min}$ and $F^i_{\max}$ are (for film i) the lower and upper bound estimates of the film inflection points, respectively.

It is worth mentioning that according to the PUMA strategy [21] (successfully used in retrieving the optical constants [1, 4, 11, 16]), the minimization problem (3) must be solved for each given trial set $(d^1_{trial}, d^2_{trial}, F^1_{trial}, F^2_{trial})$. Moreover, for each trial set of thicknesses and inflection points, the optimization method needs initial estimates for $n(\lambda)$ and $\kappa(\lambda)$. In fact, the method solves the optimization problem starting from several different initial estimations for $n(\lambda)$ and $\kappa(\lambda)$. The generation of each initial estimation is based on the approximation of $n(\lambda)$ and $\kappa(\lambda)$ by a piecewise linear function as in [2].

This amounts a lot of computer work, which increases exponentially with the number of films. For instance, for the case of a 100nm film together with a 600nm film, the trial thickness intervals would be $[10, 200]$ and $[300, 900]$, respectively (both of them with step 10 in the coarse grid). This means a total of 1220 grid points. Moreover, for the retrieval made in the spectrum interval $[1000, 2000]$, there would be 11 trial inflection points (obtained with stepsize equal to 100). This implies solving (3) $13,420$ times. If we consider that this is done for each pair of initial estimates of $n(\lambda)$ and $\kappa(\lambda)$, we conclude that at the first run, the problem (3) is solved 80,520 times.

For this reason, we implemented a parallel version of the optimization procedure described above. Paralellization is straightforward, since the optimization problems mentioned in the paragraph above can be solved independently.

4 Numerical experiments

All the experiments were run in a grid composed by a 3.00GHz Intel(R) Xeon(TM) with Hyper-threading and 2GB of RAM memory and seven 2.25GHz AMD Athlon(tm) XP 2800+ with 1GB of RAM memory. We used the language C and the Message Passing Interface (MPI) with the gcc compiler (GNU project C/C++ compiler, version 4.1.2) and the LAM MPI implementation (version 7.1.2). The program was compiled with the optimization compiler option -O4.

We performed numerical experiments with two films. Moreover, as in [2], we will consider that, for each film, $\lambda_{\text{infl}} = \lambda_{\text{min}}$ is known. We considered the case of equal and different films. Films A, B, C and D will be the computer-generated films introduced in [2], whose optical constants are described in the Appendix. In particular:

Film A: This film simulates an a-Si:H thin film with $d^{\text{true}} = 100$nm.

Film B: Identical to **Film A** except that $d^{\text{true}} = 600$nm.

Film C: This film simulates an amorphous germanium thin film with $d^{\text{true}} = 100$nm.

Film D: Identical to **Film C** with $d^{\text{true}} = 600$nm.

Moreover, g will denote the glass substrate. For example, AgB will be a system with film A on top, a glass substrate in the middle and film B on the bottom.

4.1 Identical-films systems

In this first set of experiments we considered systems with two identical 100nm *gedanken* silicon films. In particular, we considered systems with the following configurations: `AgA`, `AAg` and `gAA`. The spectral range used for the retrieval process was 570–1560nm. λ_{min} corresponds to the smallest wavelength such that the measured system transmitance is greater than or equal to 10^{-4}; λ_{max} corresponds to $\lambda_{\text{min}} + 990$nm. We use 100 measured transmitances with a wavelength step equal to 10nm.

Let us start describing the results obtained for system `AAg`. After executing Steps 1 and 2 of Algorithm 3.1, it is clear that there is no trivial way to determine "the pair of thicknesses of the grid that gives the smallest sum of squares". Figure 1 illustrates this fact. In the figure, it can be seen that any pair of thicknesses d^1 and d^2 such that $d^1 + d^2 \approx 200$nm would correspond to a system that generates the measured transmittance. As a consequence, some extra information should be given by the expert in order to choose "the right pair of thicknesses". Figure 2 shows that $d^1 = 100$nm, $d^2 = 100$nm or $d^1 = d^2$ are the kind of information that breaks the problem underdetermination. Figure 3 shows the retrievals using that $d^1 = d^2$. Note that the method retrieves a reasonable approximation of the refractive indices while it retrieves a very accurate sum (or average) of the refractive indices of both films in the system. Table 1 shows the retrieved thicknesses and the corresponding quadratic error, also for systems `gAA` and `AgA`.

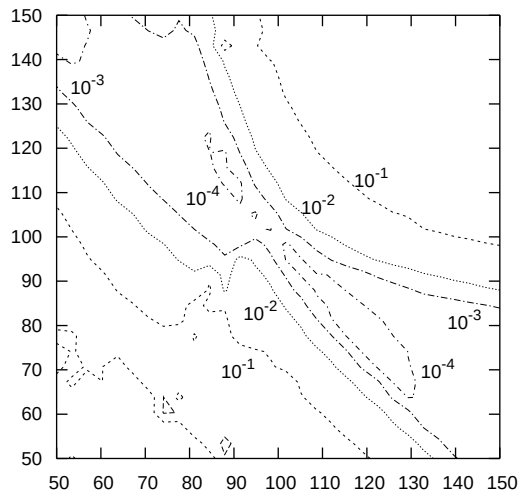


Figure 1: Level sets of the quadratic error obtained by the minimization process as a function of the trial thicknesses for the 1st and 2nd film of system AAg. The thickness of the first film is in the x-axis and the thickness of the second film is in the y-axis. Observe that the optimization process is not able to retrieve the true thicknesses. In fact, small quadratic errors appear for any pair of thicknesses whose addition is near 200nm (True thicknesses are both equal to 100nm).

Numerical experiments with system `gAA` are very similar to the ones obtained for system `AAg`. Numerical experiments with system `AgA` are also similar. Figure 4 shows the quadratic error obtained in the optimization process as a function of the trial thicknesses of the films. Note that, although in this case there is also an underdetermination, it is no related to the sum of the thicknesses of both films. Nevertheless, again, adding information related to the thickness of one of the films or saying that both thicknesses are equal is enough to promote a good retrieval. Figure 5 shows the retrievals using that $d^1 = d^2$. The retrieved thicknesses and the quadratic error are summarized in Table 1.

System	1st film		2nd film		Quadratic error
	d^{true}	d^{retr}	d^{true}	d^{retr}	
`AAg`	100	100	100	100	3.472713e-05
`gAA`	100	100	100	100	5.314831e-05
`AgA`	100	100	100	100	5.044862e-05

Table 1: Retrievals for the two-identical-films systems in the wavelenght range 540-1530nm. The extra information that both thicknesses are identical was used to break the problem underdetermination.

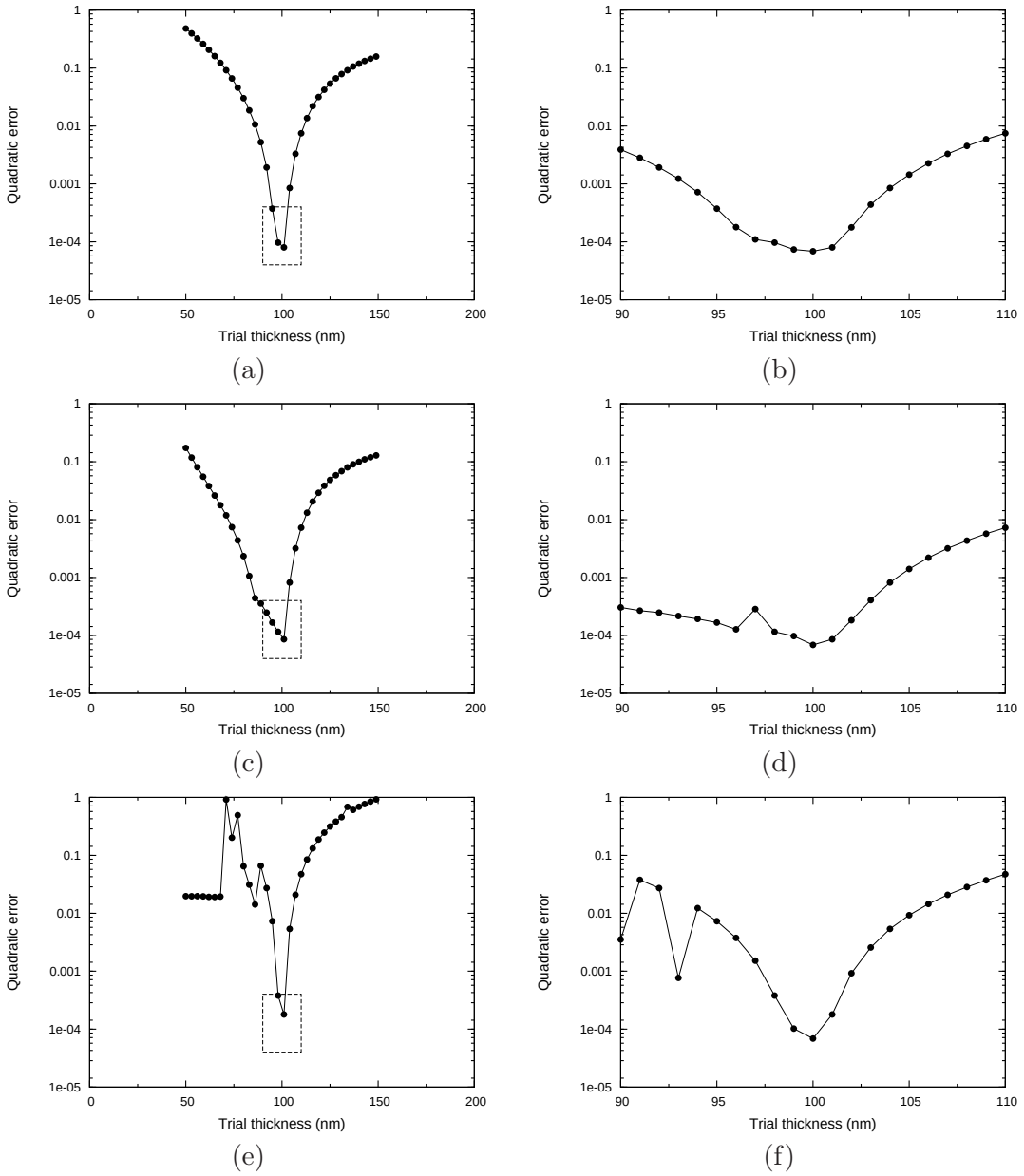
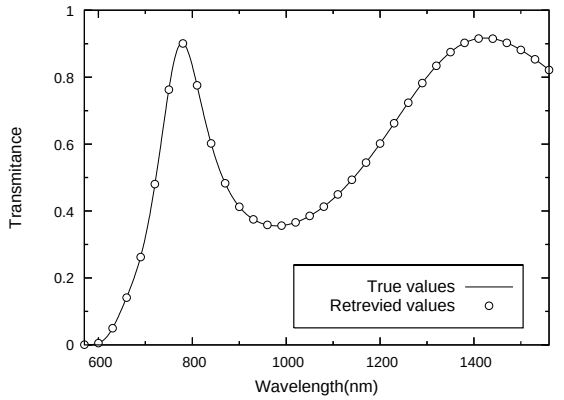
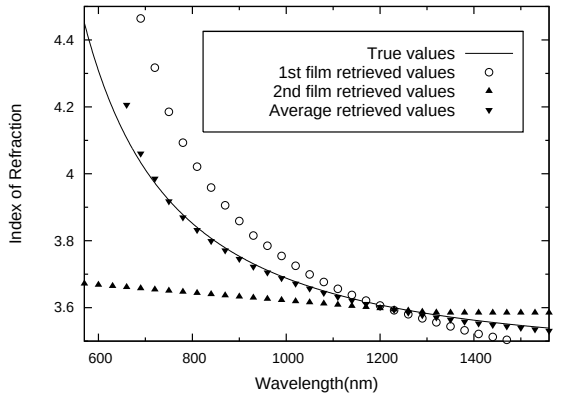


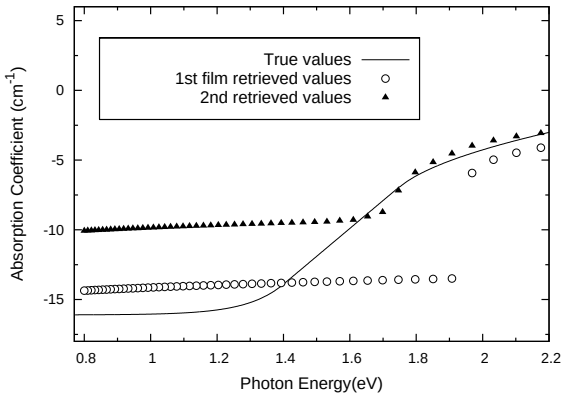
Figure 2: One-dimensional views of the quadratic error showed in Figure 1. On the left side the trial thickness step is 10nm whereas on the right hand side the refined trial step is 1nm. Graphics (a,b) represent the addition, to the optimization process, of the information that the thickness of the 1st film is 100nm. Graphics (c,d) are the same than (a,b) but for the 2nd film. Graphics (e,f) represent the addition of the information that both films have the same thickness. All of them show that the addition of any of these informations is enough for the method to retrieve the true thicknesses of both films.



(a)



(b)



(c)

Figure 3: "True" and retrieved values of (a) the transmittance, (b) the refractive indices, and (c) the absorption coefficients of the numerically generated system AAg. Graphic (b) shows that, although the method did not obtain a good retrieval of the individual indices of refraction of both films, it retrieved an accurate sum (or average) of the refractive indices.

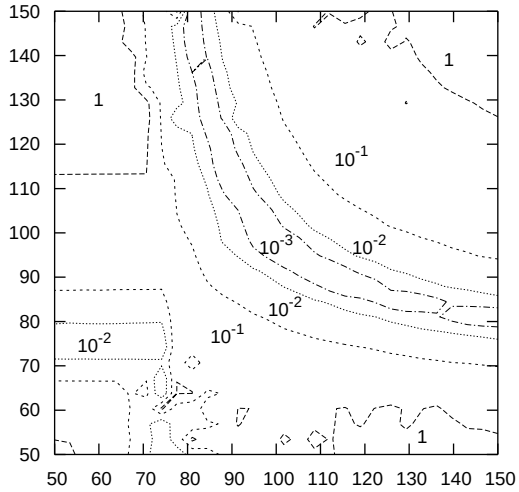
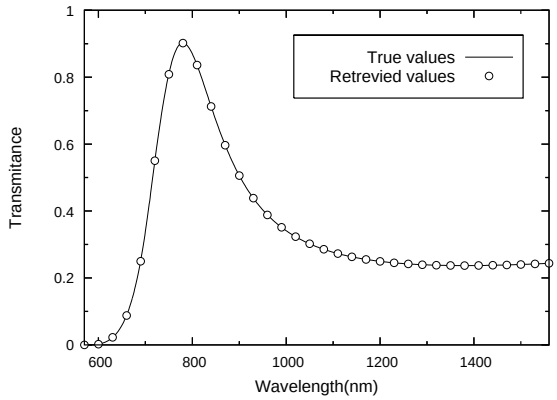


Figure 4: Level sets of the quadratic error obtained by the minimization process as a function of the trial thicknesses for the 1st and 2nd film of system AgA. The optimization process is not able to retrieve the true thicknesses: low quadratic errors appear in a curved region that resemples an hyperbola. However, as in the case of system `AAg`, it can be seen that knowing the thickness of one of the films or knowing that both films have the same thickness, the "true" pair of thicknesses can be retrieved.

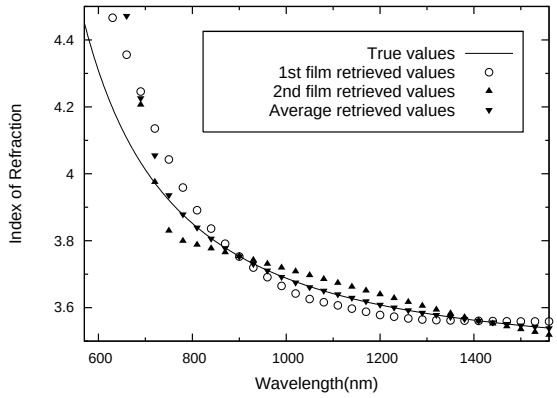
4.2 Different-films systems

In this set of tests, we considered several two-films systems combining germanium and silicon films of different thicknesses and deposited on the different sides of the glass substrate. The considered systems are: `AgB`, `BgD`, `CgB` and `CgD`. The spectral ranges used for the retrieval process were: 631–1621nm, 934–1924nm, 817–1807nm and 945–1935nm, respectively.

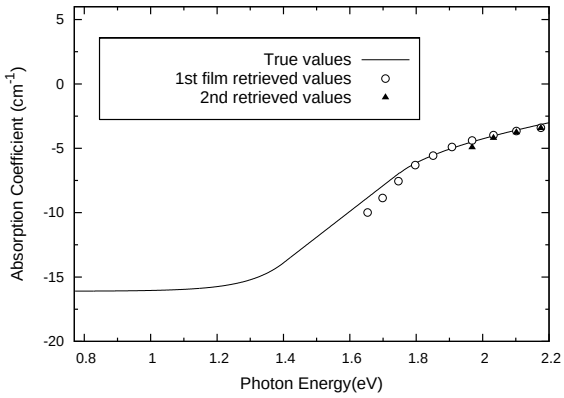
In the cases of different films, no underdeterminations appear. Roughly speaking, the true thicknesses seem to be univocally determined and the algorithm is able to recover them. Figures 6(a-d) show the quadratic errors of the minimization process as a function of the trial thicknesses for the 1st and 2nd film of systems `AgB`, `BgD`, `CgB` and `CgD`, respectively. We still observe a small underdetermination, may be due to the numerical nature of the problem (floating point arithmetic, truncation of the generated transmittance to four decimal places, local minima of the minimization problems, etc); but the region of small quadratic errors is more like a "small ball" around the "true" thicknesses instead of a "banana-shape" region as in the case of the identical-films systems experiments. Figures 7, 8, 9 and 10 show the retrievals for systems `AgB`, `BgD`, `CgB` and `CgD`, respectively. Table 2 summarizes the retrieved thicknesses and the corresponding quadratic errors.



(a)



(b)



(c)

Figure 5: "True" and retrieved values of (a) the transmittance, (b) the refractive indices, and (c) the absorption coefficients of the numerically generated system AgA. Graphic (b) shows that, although the average of the retrieved indices of refraction is more accurate than the refractive indices by themself, the refractive indices were better retrieved than in the case of system `AAg`.

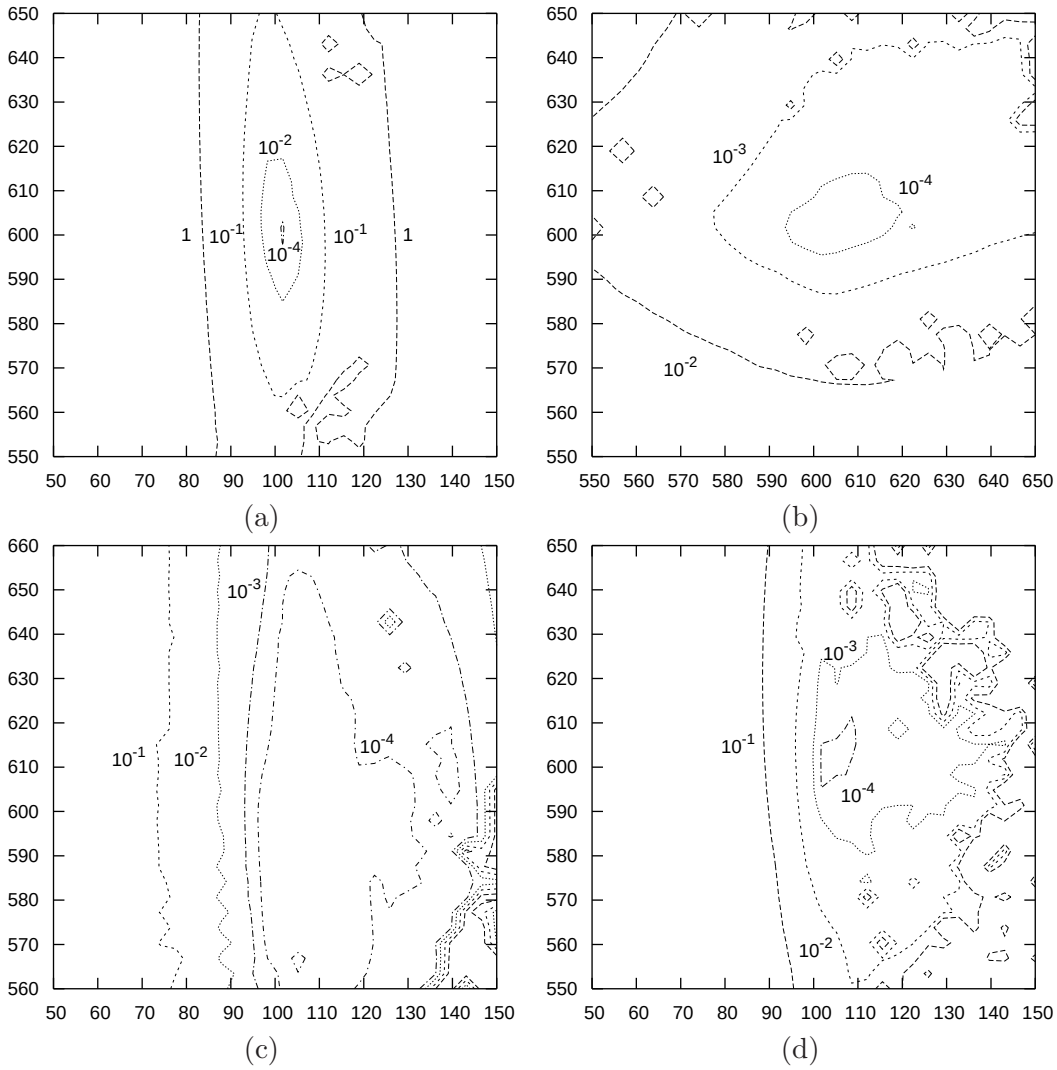
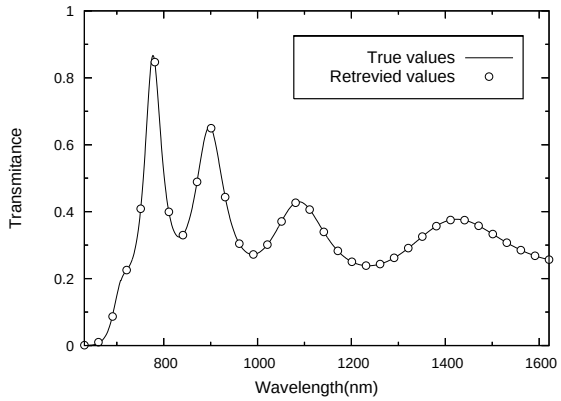
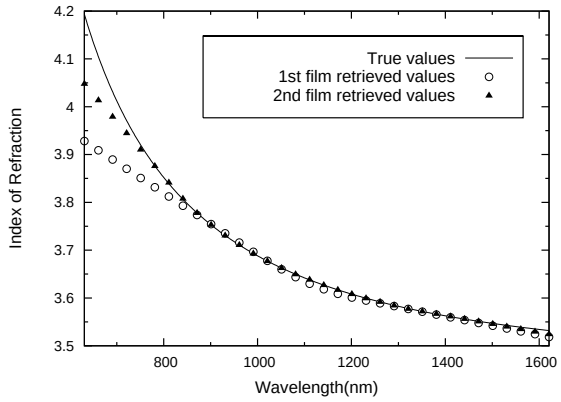


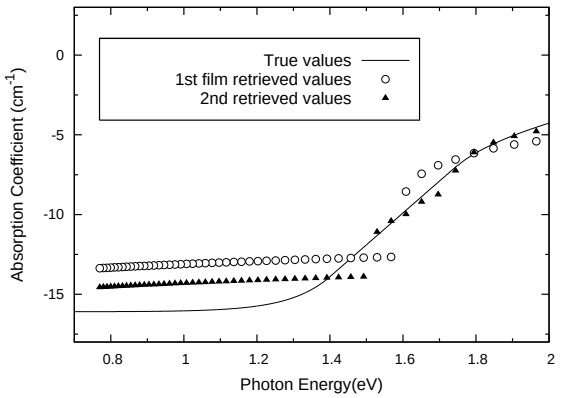
Figure 6: Level sets of the quadratic errors obtained by the optimization procedure, as a function of the 1st and 2nd film thicknesses for systems (a) `AgB`, (b) `BgD`, (c) `CgB` and (d) `CgD`. The optimization process is able to found a small region to which the pair of "true" thicknesses belongs. In several cases the "true" thicnesses are perfectly retrieved.



(a)

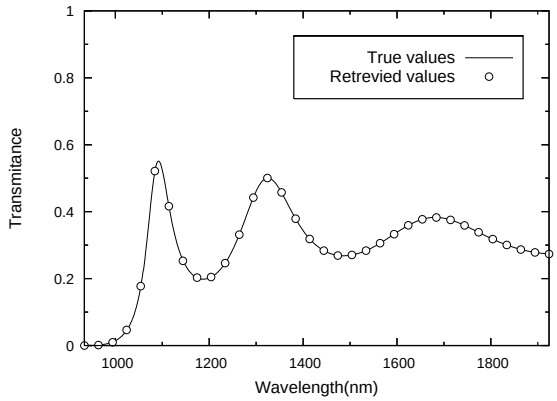


(b)

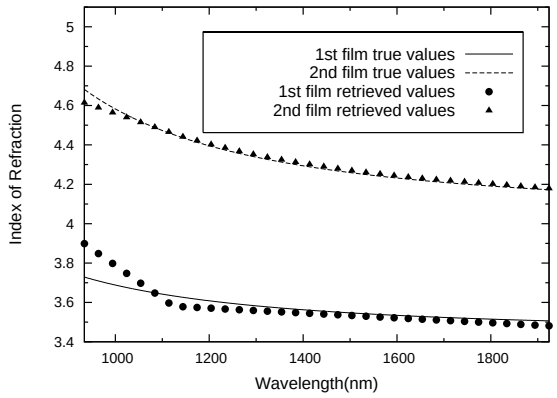


(c)

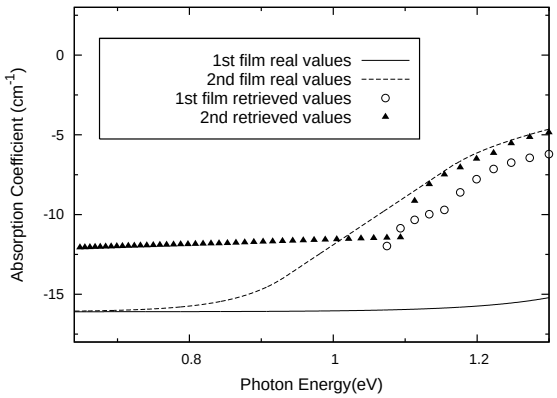
Figure 7: "True" and retrieved values of (a) the transmittance, (b) the refractive indices, and (c) the absorption coefficients of the numerically generated system AgB.



(a)

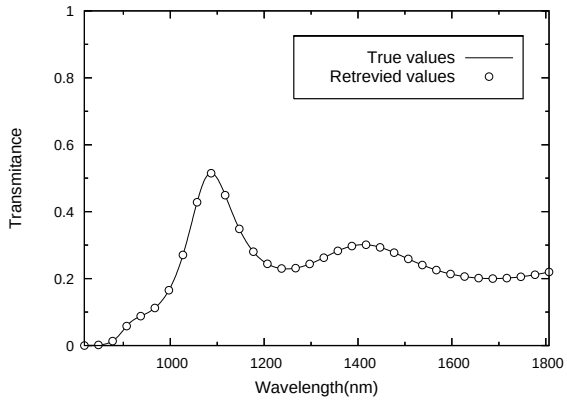


(b)

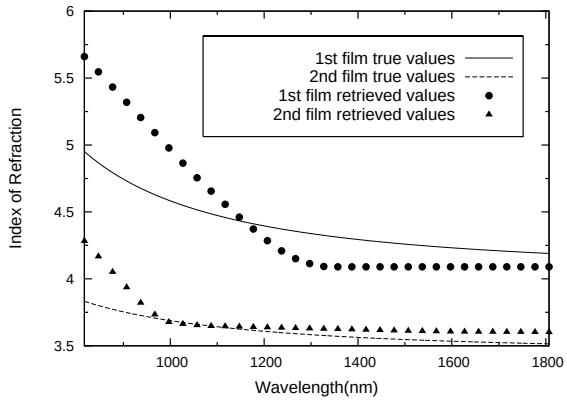


(c)

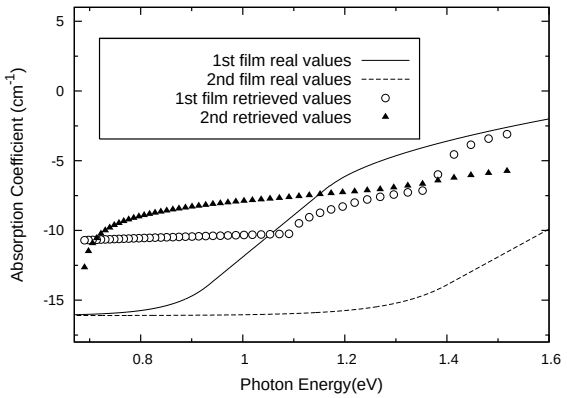
Figure 8: "True" and retrieved values of (a) the transmittance, (b) the refractive indices, and (c) the absorption coefficients of the numerically generated system BgD.



(a)



(b)



(c)

Figure 9: "True" and retrieved values of (a) the transmittance, (b) the refractive indices, and (c) the absorption coefficients of the numerically generated system CgB.

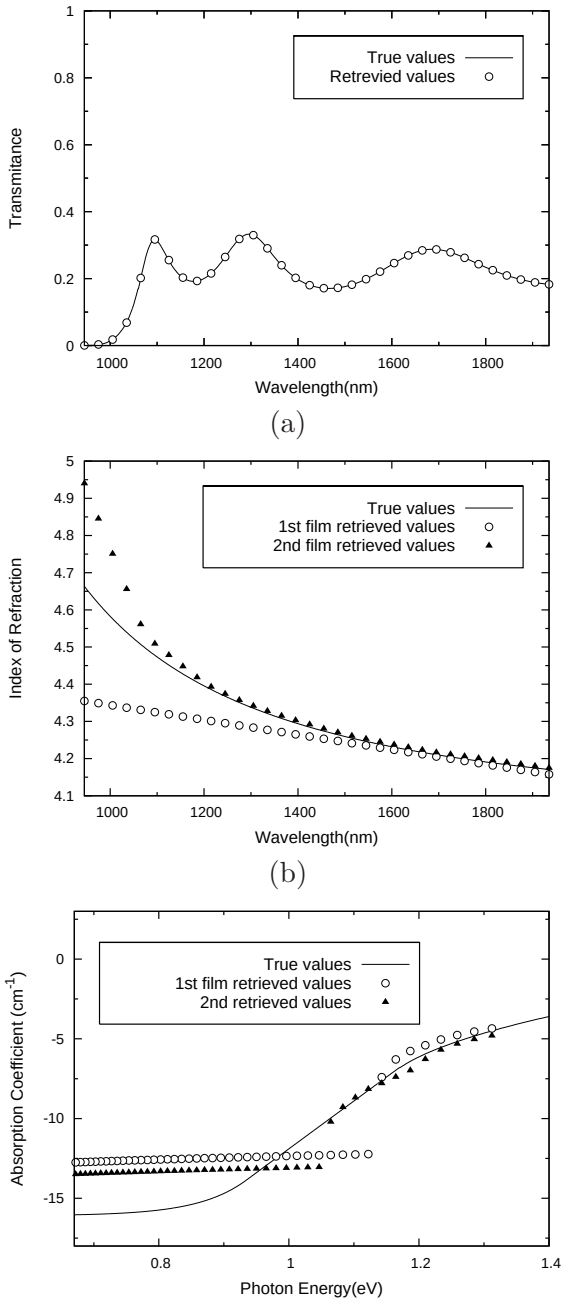


Figure 10: "True" and retrieved values of (a) the transmittance, (b) the refractive indices, and (c) the absorption coefficients of the numerically generated system CgD.

System	1st film		2nd film		Quadratic error
	d^{true}	d^{retr}	d^{true}	d^{retr}	
`AgB`	100	100	600	600	4.597773e-05
`BgD`	600	604	600	599	1.237465e-04
`CgB`	100	118	600	588	1.419527e-06
`CgD`	100	100	600	599	3.344105e-05

Table 2: Retrievals for systems `AgB`, `BgD`, `CgB` and `CgD`.

5 Conclusions

In Reverse Engineering problems, both positive and negative conclusions may be useful for technological purposes. Positive conclusions reveal that the process can be copied and negative results indicate that discovering the structure is hard and, so, that industrial secret may be maintained for longer time.

The main conclusions of the present research, concerning the retrieval of optical parameters of thin superimposed films are the following:

- Retrieval is hard when identical material films are superimposed. This is obvious when the films are deposited on the same side since, say, a film with 200 nm is indistinguishable from two superimposed films with 100 nm each. It turned out to be equaly hard in the case of films deposited on different sides of the substrate. In this case, we detected a nonlinear zone of indetermination, of hyperbolic type. Although there are no a priori reason to predict linear indetermination zones, the reasons for the hyperbolic indetermination deserve further study.

- The retrieval is good when the films are different. In this case, as shown in the level-set graphics, the indetermination is drastically reduced. The reason is that the Physical Constraints introduced in the model, although clearly insufficient for regularizing the same-film case, reduce the space of search in an efficient way in the case of two films. In other words, the constraints play, in the two-different film case, the same role played in the single-film situation.

(AQUI HABRIA QUE ACTUALIZAR ESAS CONCLUSIONES, QUE NO CORRESPONDEN TANTO A LOS EXPERIMENTOS QUE ACABAMOS DE MOSTRAR SINO A OTROS EXPERIMENTOS ANTIGUOS.) Mejor que el comandante redacte aqui las conclusiones que le parezcan.

In a general way, we can summarize the obtained results as follows:

1. For the system with two equal silicon films, the retrieved thicknesses were 100nm, when some extra information is added to thye optimization processed. Otherwise,

thicknesses such that the sum of the retrieved thicknesses is almost equal to the sum of the true ones are retrieved. This underdetermination is due to the fact that the transmittance of two (or any number of) films made of the same material depends only on the sum of all the film thicknesses but does not depend on the quantity of films nor on its individual thicknesses. Our approach can take advantage of any previous knowledge of a different range of variation of each film thickness to reduce this inherent underdetermination of the estimation problem.

Acknowledgments

Some preliminary tests of the present work were made using resources of the LCCA-Laboratory of Advanced Scientific Computation of the University of São Paulo.

Appendix

Analytical expressions used to compute the substrates and the simulated optical constants of semiconductor and dielectric films:

$$s_{glass}(\lambda) = \sqrt{1 + (0.7568 - 7930/\lambda^2)^{-1}}. \tag{20}$$

$$s_{Si}(\lambda) = 3.71382 - 8.69123\ 10^{-5}\lambda - 2.47125\ 10^{-8}\lambda^2 + 1.04677\ 10^{-11}\lambda^3. \tag{21}$$

a-Si:H
Index of refraction:

$$n^{true}(\lambda) = \sqrt{1 + (0.09195 - 12600/\lambda^2)^{-1}}. \tag{22}$$

Absorption coefficient:

$$\ln(\alpha^{true}(E)) = \begin{cases} 6.5944\ 10^{-6}\exp(9.0846E) - 16.102, & 0.60 < E < 1.40; \\ 20E - 41.9, & 1.40 < E < 1.75; \\ \sqrt{59.56E - 102.1} - 8.391, & 1.75 < E < 2.20. \end{cases} \tag{23}$$

a-Ge:H
Index of refraction:

$$n^{true}(\lambda) = \sqrt{1 + (0.065 - (15000/\lambda^2)^{-1}}. \tag{24}$$

Absorption coefficient:

$$\ln(\alpha^{true}(E)) = \begin{cases} 6.5944\ 10^{-6}\exp(13.629E) - 16.102, & 0.50 < E < 0.93; \\ 30E - 41.9, & 0.93 < E < 1.17; \\ \sqrt{89.34E - 102.1} - 8.391, & 1.17 < E < 1.50. \end{cases} \tag{25}$$

Metal oxide
Index of refraction:

$$n^{true}(\lambda) = \sqrt{1 + (0.3 - (10000/\lambda^2)^{-1}}. \tag{26}$$

Absorption coefficient:

$$\ln(\alpha^{true}(E)) = 6.5944\ 10^{-6} \exp(4.0846E) - 11.02, \quad 0.5 < E < 3.5. \tag{27}$$

In the expressions above, the wavelength λ is in nm, the photon energy $E = 1240/\lambda$ is in eV, and the absorption coefficient α is in nm^{-1}.

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