

**Determination of thickness and optical constants of amorphous silicon films
from transmittance data**

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Abstract

This work presents the application of a recently developed numerical method to determine the thickness and the optical constants of thin films using experimental transmittance data only. This method may be applied to films not displaying a fringe pattern and is shown to work for a-Si:H (hydrogenated amorphous silicon) layers as thin as 100 nm. The performance and limitations of the method are discussed on the basis of experiments performed on a series of six a-Si:H samples grown under identical conditions, but with thickness varying from 98 nm to 1.2 μm .

Modern electronic devices, such as thin-film transistors, solar cells, active matrix displays and image sensors, possess thin semiconductor layers of hydrogenated amorphous silicon (a-Si:H). For most electronic applications, the optical properties and the thickness t of these films play an important role, in the sense that they govern the device performance. The quality of the as-deposited material can be monitored in production lines through the *in-situ* determination of its optical constants (refractive index n and extinction coefficient k) and the thickness homogeneity. For that aim, ellipsometry is the most appropriate tool [1] due to the fact that it is not influenced by the adopted substrate. Alternatively, for the *ex-situ* analysis of samples grown on top of transparent substrates like glass, the use of optical transmittance is the most attractive method because optical transmission is a very easy, accurate and non-destructive measure.

The problem of estimating the thickness and the optical constants of thin films using transmission data only represents a very ill-conditioned inverse problem with many local non-global solutions. Some useful approximate solutions have been found in cases where the transmittance displays a fringe pattern in a highly transparent spectral region [2–4]. Their applicability depends on the existence of interference fringes appearing in non-absorbing regions of the transmittance spectrum. The number of fringes, in turn, depends on the sample thickness. For a-Si:H deposited on glass the minimum layer thickness needed for such analyses is of $\sim 0.7 - 1.0 \mu\text{m}$.

Two methods allowing to solve the general problem with independence of the existence of interference fringes were recently reported.[5,6] The first method [5] defines a nonlinear programming problem, the unknowns of which are the coefficients to be estimated, with linear constraints that represent prior knowledge about the physical solution. This method

was successful in retrieving the properties of computer made and of real world semiconductor films (see ref. 5). The second, [6] introduces an unconstrained formulation of the nonlinear programming model and solves the estimation problem using a method based on repeated calls to a recently introduced unconstrained minimization algorithm.[7] Numerical experiments show that the new formulation is reliable.[6] In this contribution, we apply the unconstrained formulation to a series of a-Si:H samples with thicknesses varying from 98 nm to 1.2 μm deposited under identical nominal conditions. The merits and the shortcomings of the method are discussed.

Six state of the art a-Si:H films were deposited at 250⁰C onto Corning 7059 glass substrates by the plasma enhanced chemical vapor deposition method at an excitation frequency of 13.56 MHz. The same deposition conditions were used for all of the samples, with the total deposition time being varied in order to produce similar films with different thickness. Figures 1(a) – (f) show the optical transmission spectra [$T^{meas}(\lambda)$] of the films measured at room temperature [Spectrophotometer Hitachi U–3140, scan speed of 60 nm/min]. The deposition time was diminished from (a) to (f) resulting in thinner films, as confirmed by the decreasing number of interference fringes. Note that the spectra of samples (a) and (b) display a reasonable fringe pattern in the region of weak absorption ($\lambda \geq 1000$ nm). The approximate properties of these two films can be extracted from the position and the magnitude of the maxima and the minima appearing in the interference pattern.[2–4] However, the spectra of samples (c) to (f) which possess a reduced (or absent) fringe pattern can not be analyzed with such methods.

A set of experimental data [$\lambda_i, T^{meas}(\lambda_i)$], $\lambda_{\min} \leq \lambda_i \leq \lambda_{i+1} \leq \lambda_{\max}$, for $i = 1, \dots, N$, is given, and we want to estimate $t, n(\lambda)$, and $k(\lambda)$. The problem seems highly underdetermined. In fact, for known t and given λ , the following must hold [5]: $T^{meas}(\lambda) = T^{theor}(\lambda, s(\lambda), t, n(\lambda), k(\lambda))$,

where T^{theor} is the calculated transmission of the film+substrate [3] and s the refractive index of the transparent substrate. This equation has two unknowns $n(\lambda)$ and $k(\lambda)$ and, in general, its set of solutions (n,k) is a curve in the two-dimensional $(n(\lambda), k(\lambda))$ space. Therefore, the set of functions (n,k) satisfying $T^{meas} = T^{theor}$ for a given t is infinite and, roughly speaking, is represented by a nonlinear manifold of dimension N in \mathbf{R}^{2n} . However, physical constraints (**PC**) drastically reduce the range of variability of the unknowns $n(\lambda)$, $k(\lambda)$. For example, in the neighborhood of the fundamental absorption edge of a-Si:H four of these physical constraints are: **PC1**: $n(\lambda) \geq 1$ and $k(\lambda) \geq 0$ for all $\lambda \in [\lambda_{min}, \lambda_{max}]$; **PC2**: $n(\lambda)$ and $k(\lambda)$ are decreasing functions of λ ; **PC3**: $n(\lambda)$ is convex; **PC4**: there exists $\lambda_{infl} \in [\lambda_{min}, \lambda_{max}]$ such that $k(\lambda)$ is convex if $\lambda \geq \lambda_{infl}$ and concave if $\lambda < \lambda_{infl}$. The constraints on the unknowns can be eliminated by a suitable change of variables (see ref. 6 for details).

The optimization process looks for a thickness that, subject to the physical input of the problem, minimizes the difference between the measured and the theoretical spectra, i. e.,

$$\text{Minimize } \sum_{\text{all } i} [T^{meas}(\lambda_i) - T^{theor}(\lambda_i, s, d, n_i, k_i)]^2 \quad (1)$$

The minimization process starts sweeping a thickness range Δt_R divided into thickness steps Δt_S and proceeds decreasing Δt_R and Δt_S until the optimized thickness t_{opt} is found. In the examples to follow, the starting Δt_R and Δt_S were 5 μm and 100 nm, respectively.

As seen, the most important issue of the present method is the retrieval of the real film thickness t , since it determines the $n(\lambda)$ and $k(\lambda)$ values that minimizes the quadratic error. Fortunately, the thickness of the films can be measured by independent methods and compared

with the ones obtained from the minimization process. To this aim, part of the surface of the sample films was covered with photoresist (AZ5214). The uncovered region was etched away in a reactive ion etcher apparatus and the photoresist removed. The height of the step (film thickness) was measured with a Dektak profilometer.

Figure 2 compares the thickness obtained from the analysis of transmission data (C) and that from the profilometer (M). The agreement is quite satisfactory for the whole series of samples. The relative error of the retrieved thickness with respect to the mechanical measurement is shown in the inset of Fig. 2. Note that the relative error increases with decreasing film thickness, being $\sim 10\%$ for $t = 200$ nm. The increasing difference between retrieved and measured thickness as the films go thinner may have several origins. First, the precision and accuracy of the transmitted data may not be sufficient for a perfect thickness retrieval. Second, the relative error of the mechanical measurement is larger the thinner the films. Third, there may exist a real thickness difference between the etched region and the region used for the transmittance measurements. Finally, numerical experiments, which do not contain any of the above mentioned flaws, show that the method is unable to find the true thickness for simulated a-Si:H films of $t < 75$ nm [6]. The absence of any structure in the transmittance seems to affect the retrieval process in a way not yet well understood.

Figure 3 shows the retrieved optical constants of the films. The top part of Fig. 3 displays the index of refraction n as a function of the photon energy for the whole series of samples. Different symbols are used for each film, the thickness being expressed in nanometers. Note that, for energies $E < 2.2$ eV, the index of refraction of all samples agree to a remarkable extent. This is an indication that the method works satisfactorily, in the sense that the films have been deposited under identical conditions and large variations in their properties are not expected.

At higher photon energies some deviations appear, the worst case corresponding to the $t = 98$ nm a-Si:H film.

The bottom half of Fig. 3 shows the retrieved absorption coefficient α as a function of energy ($\alpha = 4\pi k/\lambda$). The absorption coefficient is perfectly retrieved for all samples (even for the $t = 98$ nm thick film) at photon energies $E \geq 1.7$ eV. The retrieval of α at decreasing photon energy depends, as expected, on film thickness. Typically, correct values of α down to 100 cm^{-1} are retrieved for films $t \sim 1 \text{ }\mu\text{m}$. The correctness of subgap absorption values and the refractive index have been confirmed in some samples by photothermal deflection spectroscopy and ellipsometry [8]. The retrieval process of α fails when a break occurs in the smooth α vs E curve. It is followed by an almost constant value of α .

Summarizing, a numerical method to extract the optical constants and the thickness of thin dielectric films from transmission data only [6] has been tested with a-Si:H films of thickness varying in the $98 \text{ nm} < t < 1.2 \text{ }\mu\text{m}$ range. These results indicate an important improvement over other known numerical methods, the method being applicable to films not displaying any fringe pattern.

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References

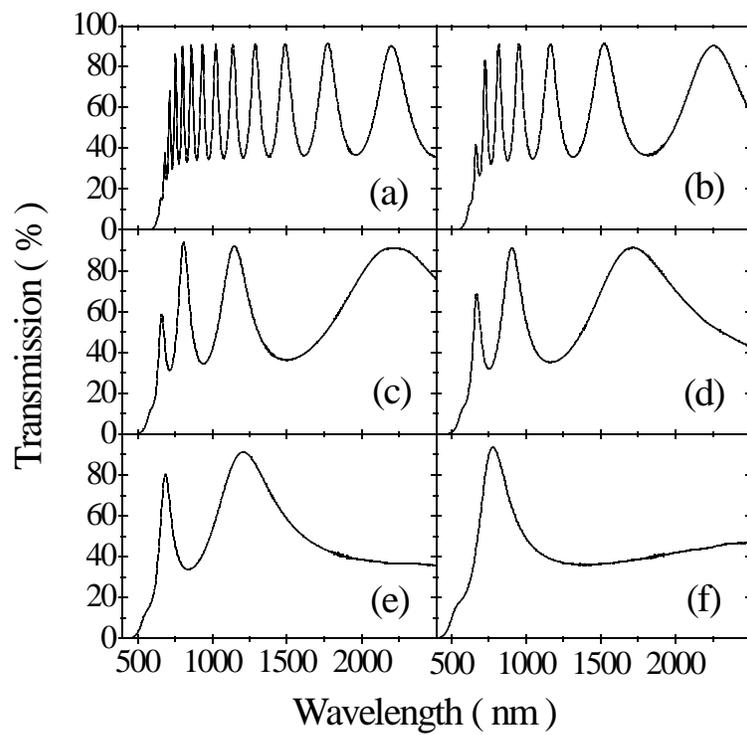
- [1] P. I. Rovira, A. S. Ferlauto, J. Koh, C. R. Wronsky, and R. W. Collins, *J. of Non-Cryst. Solids*, **266–269**, 279 (2000).
- [2] J.C. Manificier, J. Gasiot, and J.P. Fillard, *J. Phys. E* **9**, 1002 (1976).
- [3] R. Swanepoel, *J. Phys. E* **16**, 1214 (1983).
- [4] R. Swanepoel, *J. Phys. E* **17**, 896 (1984)
- [5] I. Chambouleyron, J.M. Martínez, A.C. Moretti, and M. Mulato, *Appl. Optics* **36**, 8238 (1997).
- [6] E.G. Birgin, I. Chambouleyron, and J.M. Martínez, *J. Comput. Physics* **151**, 862 (1999). [E. G. Birgin would haply provide copies of the software to the interested public. See address in authors' section].
- [7] M. Raydan, *SIAM J. Optim* **7**, 26 (1997).
- [8] E.G. Birgin, J.M. Martínez, and I. Chambouleyron, in *Optical Interference Coatings*, Opt. Soc. Am. Technical Digest **1**, 132 (1998).

FIGURE CAPTIONS

Figure 1 – Optical transmission as a function of wavelength of a-Si:H samples of decreasing thickness (from (a) to (f)) deposited under identical conditions.

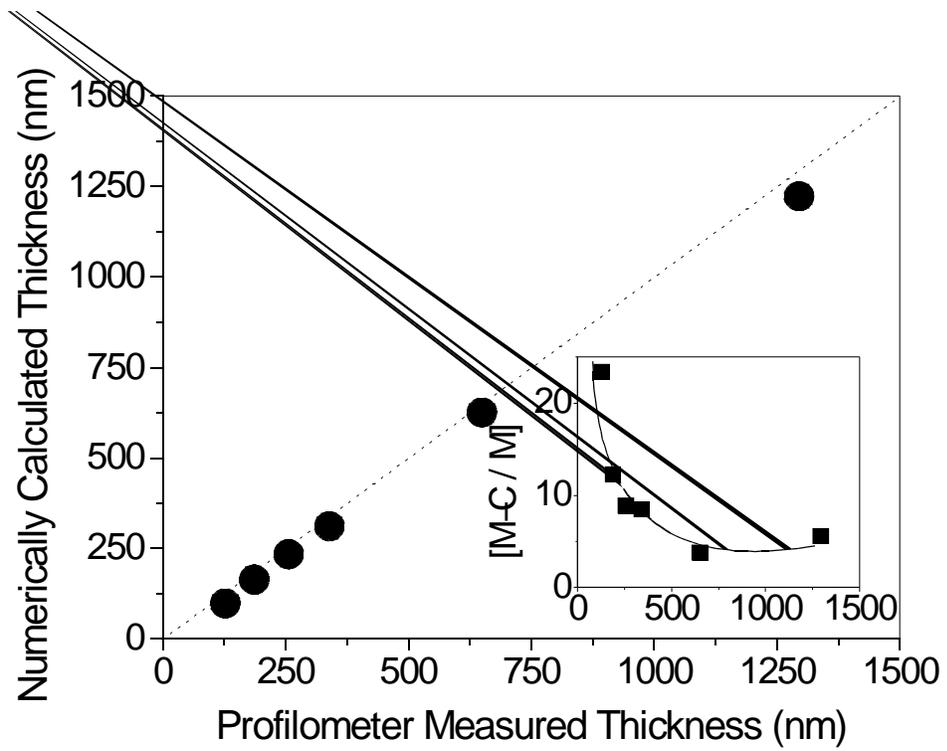
Figure 2 – Retrieved thickness *versus* thickness measured with a profilometer. The inset shows the relative error. The dotted line indicates a perfect agreement.

Figure 3 – Top: retrieved index of refraction (n) as a function of photon energy. Bottom: retrieved absorption coefficient $\alpha = 4\pi k/\lambda$. The thicknesses of the films under study are given in nm.



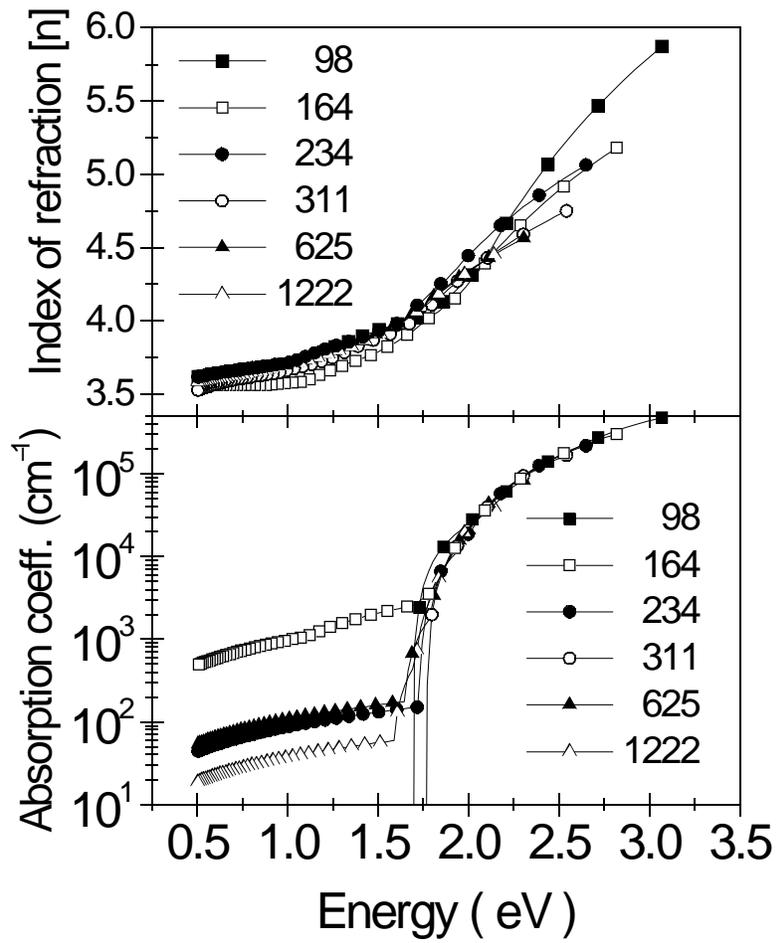
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APL – L00–1800



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APL – L00–1800



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APL – L00–1800