

Enhancing the Swanepoel Method: Precise Envelope Detection of Thin-Film Transmission Spectra

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Abstract: The Swanepoel method is a widely used optical technique for characterizing thin films through normal-incidence transmission measurements. A critical step in this approach involves extracting the upper and lower envelopes of the measured oscillatory spectrum. By analyzing the transmission spectrum and its corresponding envelopes, the Swanepoel procedure enables precise determination of the film refractive index and extinction coefficient. However, even minor inaccuracies in envelope construction can propagate significant errors into the final characterization results. To address this challenge, we present a novel physics-informed optimization algorithm for envelope detection. Our mathematical model reformulates the envelope detection problem as a global optimization task that enforces the physical properties of the Swanepoel envelopes. Extensive validation on fifty randomly generated transmission spectra demonstrates unprecedented accuracy: the method achieves root-mean-square errors (RMSE) below 0.10% for the upper envelope and 0.06% for the lower envelope (more than doubling the accuracy of current state-of-the-art approaches). Furthermore, the proposed model has been assessed with two experimental transmission spectra, demonstrating its robustness and accuracy with real noisy data. We have developed an open-source Python software package, which is available [online](#). This software includes not only our innovative envelope construction algorithm but also additional envelope drawing algorithms for comparison and an efficient implementation of the Swanepoel method, enabling complete optical characterization of thin films.

Introduction

Thin solid films are indispensable components in a vast array of optical systems and optoelectronic devices. *Semiconductor* thin films are foundational in the fabrication of transistors, diodes, and photodiodes [1–4]. For instance, silicon thin films are extensively employed for cost-effective optical sensors [5–7] and solar cells [8–10] due to their efficient light-absorbing capabilities and scalable manufacturing processes. *Conductive* thin films are highly valued for their exceptional electrical conductivity and reflectivity, enabling their use in electrode fabrication, optical mirrors, protective coatings, and forming electrical connections within integrated circuits [11–14]. In particular, transparent conductive films play a crucial role in the development of touch panels and liquid crystal displays. *Dielectric* thin films, engineered with specific refractive indices and

thicknesses, create thin-film capacitors, act as insulating layers, and form anti-reflection coatings that enhance light transmission [15, 16]. Dielectric coatings are integral to optical instruments such as lenses, bandpass filters, dichroic mirrors, and beamsplitters, providing precise control over light propagation and wavelength selection [17].

The manufacturing processes of the thin film material critically influence their optical properties [18, 19], which in turn affect the performance of the target devices. Therefore, precise determination and control of these properties are essential for optimizing the mentioned optoelectronic devices and optical systems. By performing optical characterization of thin films, we can obtain their refractive index and extinction coefficient, denoted as $n(\lambda)$ and $k(\lambda)$, respectively. These wavelength-dependent optical properties combine to form the complex refractive index ($\mathbf{n} = n + ik$) or the complex dielectric function ($\epsilon = \mathbf{n}^2$). The dielectric function offers insights into the optoelectronic properties of the film material and allows for precise quantification of the electronic transitions. Therefore, one can extract information about critical parameters such as bandgap energy [20–22], molecular disorder [23], and charge mobilities [24].

A myriad of techniques exist to determine the optical properties of thin solid films. Spectroscopic analyses are common [25–27] for characterizing materials across a broad spectral range (UV-VIS-NIR), employing transmittance, reflectance, or ellipsometric measurements. The present study focuses on characterizations derived solely from normal-incidence transmission spectra, which are optimal for assessing material properties at photon energies below the optical bandgap, where moderate to low absorption enables highly sensitive transmission data. Typically, the thin-film material is deposited on a thick glass substrate with negligible absorption ($k_s \approx 0$) and a near-constant refractive index (n_s) in the spectral region of interest (ROI). Before the thin-film preparation, the transmittance of the substrate alone, denoted $T_s(\lambda)$, is sequentially collected over different wavelengths using a spectrophotometer, allowing us to easily account for the effect of the substrate when analyzing the whole sample. As illustrated in Fig. 1a, the transmittance of the complete sample (thin film over the substrate), $T(\lambda)$, is subsequently measured.

The Swanepoel method and other characterization techniques: In 1983, Ryno Swanepoel [28] introduced an numerical procedure, widely known nowadays as the *Swanepoel method* or the *Envelope method*, to determine the thin-film thickness d and its optical functions (n and k) at specific wavelengths. These particular wavelength of interest are called *tangent points* (see Fig. 1c), as they appear where the transmission spectrum intersects (touch but not cross) its upper or lower envelopes. Although earlier envelope-based approaches had been developed before Swanepoel [29–31], his contribution significantly enhanced the precision and applicability of the technique, leading to a widespread algorithm extensively used today. Renowned for its simplicity, reliability, and computational efficiency [32], the Swanepoel method operates in the order of a few seconds on standard computers, making it ideal for rapid mass characterization of samples. Additionally, it is considered a “model-free” method, meaning that it does not rely on pre-established optical dispersion models for $n(\lambda)$ and $k(\lambda)$.

This method analyzes the interference patterns created by a quasi-monochromatic beam as it passes through a thin film, where the patterns result from the superposition of multiple internal reflections within the film (see Fig. 1b). For the desired etalon (Fabry-Perot) effect to manifest prominently within the thin film, the coherence length of the beam must exceed the film thickness (typically on the micrometer scale), denoted d . This ensures that multiple internal reflections within the film lead to significant constructive and destructive interference, depending on the wavelength. Consequently, the transmission spectrum $T(\lambda)$ exhibits characteristic sinusoidal oscillations with distinct peaks and valleys, as illustrated in Fig. 1c. The Swanepoel method exploits these spectral oscillations to accurately determine the film properties. Note that in order to prevent the substrate from generating its own etalon effects, the coherence length must be

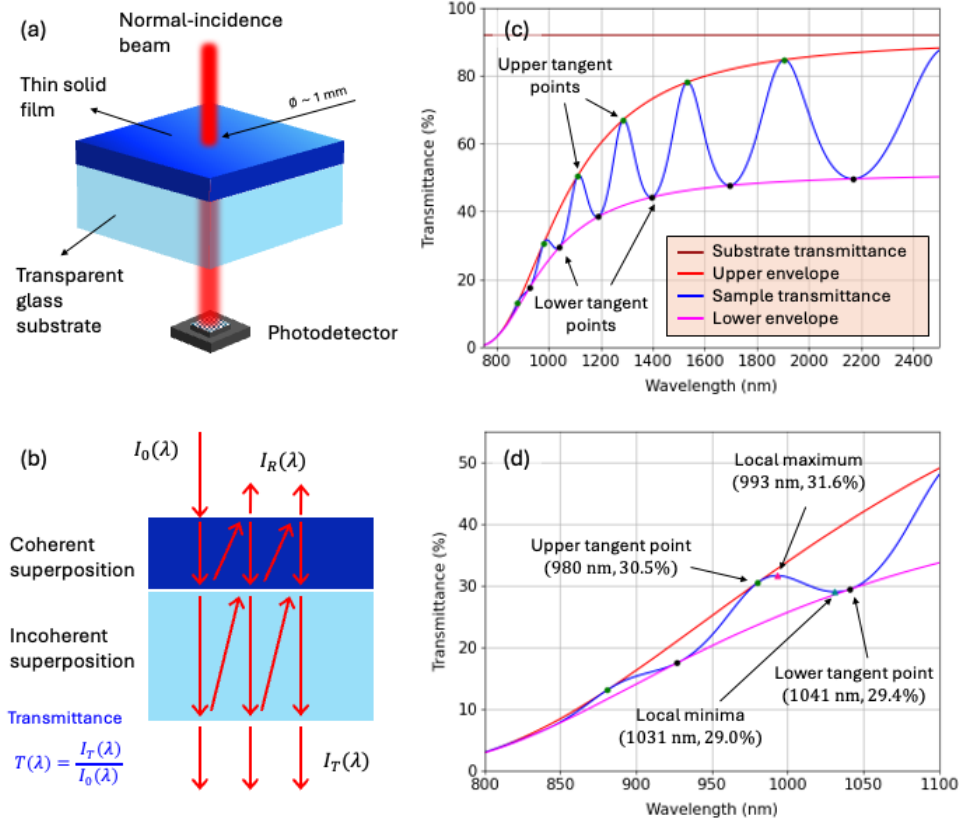


Fig. 1. (a) Schematic of the sample geometry, comprising a thin layer deposited on a glass substrate. (b) Multiple internal reflections within the thin film and the substrate. The total transmittance is measured sequentially throughout different wavelengths. (c) Simulated transmission spectra for the full sample and for the substrate alone. The ground-truth upper and lower envelopes, along with their tangent points, are indicated. (d) Magnified view of the strongly absorbing spectral region. The upper and lower tangent points are sometimes not associated with a nearby local extremum (first two on the left), or occur at positions significantly far from the local extrema (last two on the right).

set shorter than the substrate thickness¹ (typically on the millimeter scale), denoted d_s . This condition ensures that any multiple reflections within the substrate do not contribute to coherent interference patterns, resulting instead in an incoherent superposition of the beams. The exact value of d_s is therefore not relevant for the characterization of the sample.

Since its inception, the Swanepoel method has served as a key computational method for the analysis of thin-film optical analysis, inspiring numerous enhancements that have significantly broadened its applicability. For instance, shortly after introducing his original algorithm, Swanepoel himself extended the methodology in 1984 [34], enabling the analysis of films with tilted planar-specular surfaces. The algorithm can then apply to samples with non-uniform thickness, generally characterized by a wedge Δd . In 1986, Kushev *et al.* generalized the

¹As the coherence length increases with wavelength, it may eventually exceed the substrate thickness at longer wavelengths. This can lead to very high-frequency oscillations [33], causing aliasing when the oscillation frequency surpasses the spectral sampling rate used in the experiment. Such aliasing manifests as characteristic noise at the spectrum's end if the experiment is not carefully calibrated.

106 envelope method to the field of reflectometry [35], enabling the determination of thin-film optical
107 properties from normal-incidence reflectance measurements. In 1995, Nowak [36] investigated
108 the effects of realistic band-limited incident beams with either linear or Gaussian spectral profiles,
109 further refining the accuracy of the method. Later, Wu *et al.* (2008) [37] extended the method to
110 analyze inhomogeneous films with a linearly graded refractive index from the substrate interface
111 to the film surface. Jin *et al.* contributed two very significant advancements in 2017. First, they
112 analyzed the spectral regions in which the film presents strong absorption [38], where the original
113 Swanepoel method produced substantially less accurate solutions. Then, they expanding the
114 algorithm to determine the refractive index n and extinction coefficient k at arbitrary wavelengths,
115 not just at the mentioned tangent points [39].

116 Besides the Swanepoel method, the *inverse synthesis* approach also stands out as an alter-
117 native leading algorithm [40–43]. This method involves fitting the experimental transmission
118 measurements with a simulated transmission curve, which rely on specific pre-established
119 dispersion models for the refractive index $n(\lambda)$ and the extinction coefficient $k(\lambda)$. Although
120 generally more precise over a broad continue spectral range, the inverse synthesis approach is
121 also considerably more complex, demands higher computational resources, and does not always
122 guarantee physically meaningful characterizations (as explained in the next section). Moreover,
123 it should be remarked that there is not a universal dispersion model that successfully applies
124 to all materials and over the infinite spectral range. Instead, one needs to carefully study the
125 film material and its electronic transitions beforehand in order to decide the optimal dispersion
126 models and the number of oscillators [44]. Given these uncertainties inherent to the inverse
127 synthesis method, it is always advisable to use the Swanepoel method to verify and compare
128 results, as commonly practiced in the literature [45, 46]. Besides the envelope method and the
129 inverse synthesis, further computational approaches are emerging. For instance, there is a Deep
130 Learning architecture that directly predicts a film properties from transmission data [47]. Another
131 recent technique employs a digital twin [48] to numerically simulate wave propagation through
132 the spectrophotometer.

133 **Envelope detection algorithms:** The Swanepoel method assumes precise knowledge of both
134 the upper and lower envelopes of the transmission spectrum (refer to Fig. 1b). In practice,
135 accurately identifying these envelopes is a significant challenge on its own. The accuracy of the
136 Swanepoel method is highly dependent on the precise determination of these envelopes, as any
137 discrepancies in their construction propagate through the entire algebraic procedure, ultimately
138 affecting the reliability of the film characterization. In 1991, Marjorie McClain *et al.* [49]
139 addressed this problem by introducing a robust iterative algorithm for envelope construction. This
140 seminal work has since established the McClain algorithm as the standard approach, extensively
141 utilized in the literature [50–52]. The McClain algorithm is both efficient and reasonably
142 accurate in practical applications. It determines the envelopes using B-spline interpolation of
143 the mentioned tangent points, which are seen in Fig. 1c. As anticipated, the accuracy of this
144 interpolation-based method improves with an increasing number of interpolation nodes, requiring
145 at least four spectral oscillations with its four associated tangent points to produce reliable results.
146 Beyond the original McClain algorithm, several other interpolation-based methodologies have
147 been proposed to enhance envelope detection [53–56].

148 Alternative approaches have been developed to address spectra with limited number of
149 oscillations, sometimes displaying only two or three tangent points. A common strategy in
150 such scenarios involves fitting the envelopes by connecting local extrema (maxima for the upper
151 envelope and minima for the lower envelope) using predefined exponential [57, 58] or parabolic
152 functions [59]. However, it should be mentioned that, although the tangent points typically lie
153 near the extrema of the transmission spectrum, they do *not* coincide precisely. Indeed, observe
154 that the film absorption induces a decay in the transmittance curve as wavelengths decrease and
155 approximates the optical band gap, causing the tangent points to shift slightly away from the

extrema, as seen in Fig. 1d. In the regions of strong film absorption (where the transmission spectrum remains low) the tangent points may not correspond to any local minimum or maximum at all, as illustrated by the first lower and upper tangent points of the simulated spectrum, in Fig. 1d. Consequently, the mentioned parabolic and exponential fits often lead to noticeable errors in the constructed envelopes. A recently proposed deep learning-based method [60] developed by our team shows promise in accurately determining envelopes for transmission spectra, even in these challenging scenarios with as few as two or three tangent points. However, this approach has so far been validated only with simulated data and not with real, noisy experimental measurements.

Enhancing the accuracy of envelope computation remains a significant and ongoing challenge in the field. In the present work, we propose a novel interpolation-based algorithm for the precise determination of Swanepoel envelopes. Our approach integrates the physical properties of the Swanepoel envelopes into a global optimization framework, which is then efficiently solved using an advanced optimizer. We validated our method using fifty computer-generated transmission spectra, achieving a root-mean-square error (RMSE) of less than 0.10% for the upper envelope and below 0.06% for the lower envelope. These results demonstrate a significant enhancement in accuracy compared to existing methods, reducing errors by more than half with respect to the standard McClain algorithm, as detailed in the subsequent comparison section. While our proposed method is more computationally expensive than the existing algorithms, it still performs in a reasonable timeframe and runs in less than a minute using standard computer hardware.

Furthermore, we have integrated our innovative envelope construction algorithm with an automated adaptation of the original Swanepoel method within a user-friendly Python package named `swanpy`. This open-source software is publicly accessible at this [link](#). Note that `swanpy` does not only includes our novel envelope construction algorithm but also incorporates additional standard envelope detection techniques for comparative analysis. Our automated and efficient implementation of the Swanepoel method facilitates the comprehensive optical characterization of thin films. It is worth noting that the present work demonstrates the effectiveness of `swanpy` in practical applications by fully characterizing two real amorphous silicon (*a*-Si) samples, which were previously analyzed by our team [46] and used here as a benchmark.

Thin film transmission equation and inverse-synthesis challenge

As discussed earlier, the inverse synthesis method requires a simulator to reproduce the transmission curve, which is then fitted to experimental data. To develop such a simulator, we begin with the theoretical expression for normal-incidence transmittance, derived from the Fresnel equations [61]. Following extensive derivations in [33], the final formula relates the wavelength λ and the film's optical properties (n, k, d) to the transmittance. Assuming a uniform, isotropic, and homogeneous film deposited on a transparent substrate with a known refractive index n_s , the resulting expression is:

$$T^{\text{sim}}(\lambda; n, k, d) = \frac{A'x}{B' + x(C'_1 \sin \varphi - C'_2 \cos \varphi) + D'x^2}, \quad (1)$$

where

$$\alpha = 4\pi k/\lambda, \quad (2a)$$

$$x = e^{-\alpha d}, \quad (2b)$$

$$\varphi = 4\pi nd/\lambda, \quad (2c)$$

$$A' = 16(n^2 + k^2)n_s, \quad (2d)$$

$$B' = ((n+1)^2 + k^2)((n+1)(n+n_s^2) + k^2), \quad (2e)$$

$$C'_1 = 2k(2(n^2 + k^2 - n_s^2) + (n^2 + k^2 - 1)(n_s^2 + 1)), \quad (2f)$$

$$C'_2 = 2(n^2 + k^2 - 1)(n^2 + k^2 - n_s^2) - 4k^2(n_s^2 + 1), \quad (2g)$$

$$D' = ((n-1)(n-n_s^2) + k^2)((n-1)^2 + k^2). \quad (2h)$$

193 Observe that the refractive index of the substrate, n_s , is known because it can be computed
194 beforehand from the transmission of the substrate alone, T_s , using the equation [33]:

$$n_s = 1/T_s + \sqrt{1/T_s^2 - 1}. \quad (3)$$

195 It should also be emphasized that α (1/cm) in Eq. 2a corresponds to the absorption coefficient.
196 Additionally, the term x in Eq. 2b denotes the a fraction of the transmitted intensity: this
197 parameters is calculated from the Lambert-Beer law [61] and ranges from 0 to 1, expressing the
198 amount of light that passes through the film in one single pass (not accounting for multiple round
199 trips of the beam within the film). Lastly, the two trigonometric functions in the denominator of
200 Eq. 1 depend on the phase φ and account for the Fabry-Perot thin-film interferences, corresponding
201 to the low-frequency oscillations noticeable in the transmission spectrum.

202 One could naively develop a least-squares regression program to fit the experimental trans-
203 mission spectrum $T(\lambda)$ to the theoretical model $T^{\text{sim}}(\lambda; n(\lambda), k(\lambda), d)$, thereby determining the
204 film's optical and geometrical properties $n(\lambda)$, $k(\lambda)$, and d . However, n and k are intricate
205 wavelength-dependent functions and not simple constants. Multiple combinations of n and k can
206 produce the same theoretical transmission spectrum, making this fitting problem *ill-posed* in
207 nature. As Kushev and Zheleva [35] realized in 1986, “the system is satisfied by many solutions
208 and it is difficult to identify the real physical one”.

209 The *inverse synthesis* method takes this fitting idea a step further and eases the problem
210 by assuming some pre-defined dispersion models for the optical functions $n(\lambda)$ and $k(\lambda)$.
211 Consequently, these complicated optical functions are expressed in terms of just a few real
212 coefficients. For instance, one can employ the simple Wemple-DiDomenico (WDD) dispersion
213 equation [62] for n and the Urbach rule [63] for the absorption coefficient α (the extinction
214 coefficient k can then be derived using Eq. 2a). We then have the following formulas:

$$n(E; E_0, E_d) = \sqrt{\frac{E_0 E_d}{E_0^2 - E^2} + 1}, \quad (4a)$$

$$\alpha(E; \alpha_0, E_u) = \alpha_0 \exp\left(-\frac{E}{E_u}\right). \quad (4b)$$

215 The parameter E_0 (eV) represents the oscillator energy in a single-oscillator electron model,
216 corresponding to the average energy of electronic interband transitions. E_d (eV) is the dispersion
217 energy, which quantifies the strength of interband optical transitions and provides an extra degree
218 of freedom to account for the refractive index value as the photon energy approaches zero $E \rightarrow 0$.
219 The parameter α_0 (1/cm) defines the absorption coefficient in the limit of zero photon energy.
220 The Urbach energy, denoted as E_u (eV), characterizes the exponential decay of the absorption

coefficient with decreasing photon energy below the bandgap, indicating the degree of structural disorder in amorphous materials responsible for sub-bandgap absorption. Please note that Eqs. 4a-4b can be similarly expressed as functions of wavelength using the Planck-Einstein relation $E = hc/\lambda$, where h is Planck's constant and c is the speed of light in vacuum.

The combined WDD-Urbach model offers a foundational estimate of the electronic transitions in thin-film materials. This model is primarily applicable to amorphous materials with two main energy levels, encompassing a single dominant electronic transition between the valence and conduction bands, which defines the bandgap energy. However, it disregards weaker transitions that may play a significant role in crystalline materials. Furthermore, this dispersion model is limited to specific spectral regions, particularly for photon energies that are well below the optical bandgap but remain sufficiently separated from phonon resonances in the near-infrared range. In the simulated example illustrated in Fig. 1, we used the following parameter values: $E_0 = 4.28$ eV, $E_d = 30.45$ eV, $\alpha_0 = 269.46 \text{ mm}^{-1}$, $E_u = 229.18$ meV, and $d = 1323$ nm.

Employing more precise models that are consistent with the Kramers-Kronig relations between n and k increases computational complexity considerably. This complexity is particularly evident when utilizing various modifications and adaptations of the Tauc-Lorentz-Urbach (TLU) [46, 64–66] and Cody-Lorentz-Urbach (CLU) [64, 67, 68] models, which are valid across the entire spectral range. These advanced models, enhanced with numerous refinements, necessitate extensive computations and introduce additional subtle and intricate variables into the simulator.

Regardless of the optical dispersion model chosen, the inverse synthesis approach enables the simplification of the transmittance formula $T(\lambda; n(\lambda), k(\lambda), d)$ from Eq. 1 in terms of only a few input coefficients. In our case, the WDD-Urbach model allows us to rewrite the simulated transmission curve as a function of $(E_0, E_d, \alpha_0, E_u, d) \in \mathbb{R}^5$. With these scalar values, we can establish the following least-squares optimization problem:

$$\begin{aligned} \text{minimize} \quad & C(E_0, E_d, \alpha_0, E_u, d) = \text{RMSE}(T, T^{\text{sim}}) = \sqrt{\frac{\sum_{i=0}^N [T(\lambda_i) - T^{\text{sim}}(\lambda_i; E_0, E_d, \alpha_0, E_u, d)]^2}{N}}, \\ \text{subject to} \quad & \begin{cases} E_0 \in [a_1, b_1], & E_d \in [a_2, b_2], \\ \alpha_0 \in [a_3, b_3], & E_u \in [a_4, b_4], \\ d \in [a_5, b_5]. \end{cases} \end{aligned} \tag{5}$$

The cost function C quantifies the discrepancy between the predicted and experimental spectra across the discrete wavelengths within the spectral region of interest (ROI). Achieving cost values below 1-1.5% typically indicates a good fit between the simulated and measured data [46, 69]. However, the acceptable threshold for the cost function depends on the spectral range length and the specific characteristics or noise level of the measurements. Note that in Eq. 5, the box constraints $[a_i, b_i]$ define the acceptable ranges for the parameters, which vary depending on the specific thin-film material under investigation.

Although this inverse synthesis approach is a popular choice for optical characterization, it is not without limitations. For instance, there is the crucial task of setting feasible constraint ranges for a_i and b_i , as the computational effort increases notably when these ranges are broadened. Furthermore, the inverse problem is inherently non-convex in nature, marked by numerous local minima and maxima, and necessitating the use of sophisticated global optimization algorithms. These global optimizers are often affected by the curse of dimensionality, resulting in substantially increased computational costs as the number of variables grows. Additionally, in practical scenarios with noisy data and approximated simulation models, these algorithms can still produce solutions that are mathematically acceptable (satisfying constraints and exhibiting low cost

values) but physically inaccurate, corresponding to local minima rather than the global optimum. To mitigate the risk of converging to suboptimal local minima, it is recommended to execute these optimization algorithms multiple times with different initial points or random seeds and to compare the resulting solutions. This approach enhances the likelihood of identifying the most accurate and reliable characterization of the system.

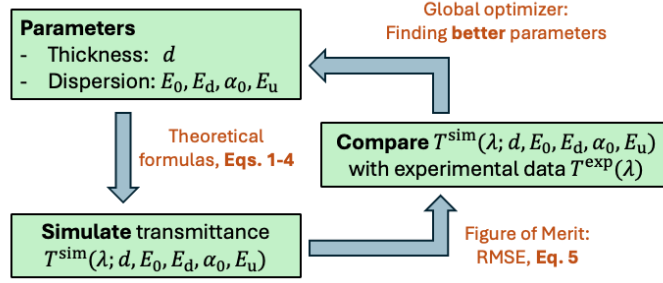


Fig. 2. Random initial guesses for the film parameters (such as thickness and the coefficients of the optical dispersion model) are selected. A theoretical transmittance spectrum is calculated from these parameters via Eq. 1. The simulated spectrum is then compared to the experimental spectrum, and the residual error is quantified using the cost function (RMSE) defined in Eq. 5. A global optimization algorithm iteratively adjusts the parameters to minimize this residual error. This process repeats until the optimal parameters that yield the best fit between the simulated and experimental spectra are found.

The runtime of the inverse synthesis method is influenced by several factors, including the particular dispersion model employed and its number of variables, the choice of the global optimizer and its hyperparameters (such as the number of iterations or initial seeds), the range of the box constraints, and the number of times the optimization is executed to corroborate results. Consequently, solving the inverse problem described by Eq. 5 can become a computationally intensive task, sometimes requiring hours of manual fine-tuning and computation.

For a later comparison of our improved Swanepoel method, we use now the inverse synthesis method to characterize two real spectra. Specifically, two *a*-Si samples were prepared using radio-frequency magnetron sputtering (RFMS) on top of a transparent Corning Eagle XG glass substrate. The target p-type silicon had a 5N purity and a density of 2.32 g/cm³. During thin-film deposition, the RFMS chamber was maintained at room temperature (25 °C) with an RF power of 525 W. The deposition rates were 1.269 nm/s for sample #1 and 1.339 nm/s for sample #2. The chamber pressures were 4.4 Pa and 3.2 Pa, and the argon gas flow rates were 70 sccm and 50 sccm for samples #1 and #2, respectively.

Transmission measurements of both the substrate alone and the full sample were collected using an Agilent Cary 5000 double-beam spectrophotometer, covering the UV-VIS-NIR range from 300 to 2500 nm. The initial spectral range (up to 700 nm) was cropped out to avoid the interval where the substrate exhibits considerable absorption and where the thin film shows very strong absorption (leading to a near-zero transmission), which provides no useful information for characterization. The fitting problem was then solved using the Simulated Dual Annealing algorithm, an efficient global optimizer available in the Python *scipy* package [70]. Figure 3 illustrates the agreement between the experimental and simulated spectra, with root mean square errors (RMSE) of 0.85% for sample #1 and 0.98% for sample #2. The bottom panel of the figure displays the residual disagreement or fitting error, defined as $T^{\text{exp}} - T^{\text{sim}}$. Notably, in the NIR region beyond 2100 nm, where the substrate exhibits slight absorption, a stronger disagreement is observed in Fig. 3a.

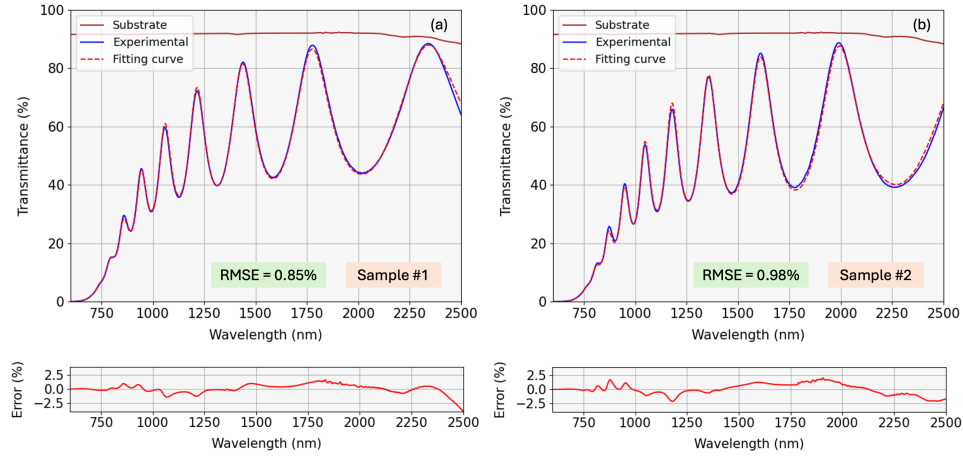


Fig. 3. Comparison of experimental transmission measurements with simulated transmission curves for (a) sample #1 and (b) sample #2 of amorphous silicon, obtained using the inverse synthesis method. The bottom panels illustrate the residual differences or error between the experimental and simulated data, defined as $T^{\text{exp}} - T^{\text{sim}}$.

293 The optimal parameters obtained from the inverse synthesis method for samples #1 and #2 are
 294 summarized in Table 1. Initially, the points for the optimization were randomly chosen within the
 295 specified bounds for each parameter. In this particular case, the optimization process required
 296 only a few minutes of computation time and manual adjustments of the bounds, thanks to the
 297 relatively low dimensionality of the simplistic models for n and k employed here for illustrative
 298 purposes.

Table 1. Optimized parameters for amorphous silicon samples obtained from the inverse synthesis method. The initial bounds for each parameter are also provided.

Parameter	Unit	Lower Bound	Upper Bound	Sample #1	Sample #2
Thickness d	nm	500	1500	1117	1160
Energy gap E_0	eV	3.2	5.0	3.22	3.21
Dispersion energy E_d	eV	25	35	27.96	33.28
Absorption coefficient α_0	cm^{-1}	0.1	0.5	0.225	0.186
Urbach energy E_u	eV	0.1	0.3	0.247	0.234

299 Automated Swanepoel method

300 As previously noted, the Swanepoel method provides a more straightforward alternative to the
 301 inverse synthesis approach. It relies on the principles of Fabry-Perot interference and employs
 302 the simple algebraic interference formula to perform the optical characterization. Although the
 303 method's approximations can reduce the precision of the estimated film properties, it offers several
 304 key advantages: it requires far less computational effort, imposes no dispersion assumptions, and
 305 avoids multiple non-physical solutions. In other words, instead of encountering the ambiguity

often faced with inverse synthesis methods, the Swanepoel approach yields a unique, physically meaningful set of values for n , k , and d .

Our automated program is based on the original Swanepoel algorithm from 1983 [28], designed specifically for plane-parallel thin films of uniform thickness, composed of isotropic and homogeneous materials. As previously discussed, numerous adaptations of this algorithm have been proposed to handle more complex scenarios [34–39], and these enhancements could potentially be integrated into our software framework in the future.

In spectral regions where the sample presents medium-to-weak optical absorption, the condition $n^2 \gg k^2$ holds. These spectral regions, frequently examined in transmission spectroscopy studies, correspond to photon energies below the optical bandgap. Under this circumstance, Eq. 1 can be simplified as follows:

$$T^{\text{sim}}(\lambda; n, k, d) = \frac{Ax}{B - Cx \cos \varphi + Dx^2}, \quad (6)$$

where

$$\begin{aligned} A &= 16n^2n_s, \\ B &= (n+1)^3(n+n_s^2), \\ C &= 2(n^2-1)(n^2-n_s^2), \\ D &= (n-1)^3(n-n_s^2). \end{aligned} \quad (7)$$

In contrast with the more accurate Eq. 1, given that Eq. 6 now only comprises a single sinusoidal function, we can find the two envelopes of the oscillating transmission curve by assigning $\cos(\varphi) = 1$ for the upper envelope T_M^{sim} , and $\cos(\varphi) = -1$ for the lower envelope T_m^{sim} . These envelopes are then expressed as follows:

$$T_M^{\text{sim}}(\lambda; n, k, d) = \frac{Ax}{B - Cx + Dx^2}, \quad (8a)$$

$$T_m^{\text{sim}}(\lambda; n, k, d) = \frac{Ax}{B + Cx + Dx^2}. \quad (8b)$$

The intersection points between the simulated transmission spectrum T^{sim} and its upper envelope T_M^{sim} are identified as the upper tangent points, which are represented by λ^{M} , as shown in Fig. 1b. Similarly, λ^{m} denotes the lower tangent points, which are associated with the intersections of T^{sim} with its lower envelope T_m^{sim} . Due to the sinusoidal characteristic of Fabry-Perot oscillations, these upper and lower tangent points occur in an alternating pattern. The sorted sequence of these tangent points is expressed here as λ^{tan} .

While determining the simulated envelopes of a simulated transmission curve is straightforward, following their definition from Eq. 8 (as done for the initial Fig. 1), identifying the Swanepoel envelopes of an *experimental* curve poses a significant challenge. The Swanepoel method assumes that the true envelopes, T_M and T_m , of a measured transmission spectrum T have already been (somehow) accurately determined. Based on this assumption, the optical properties n and k are extracted using a series of physically meaningful equations, evaluated exclusively at the tangent points. Below, we detail our automated step-by-step procedure for implementing the Swanepoel method, which is summarized in Fig. 4.

Preliminary estimation of n_1 and d_1

In this preliminary step, we carry out a rough estimation of the refractive index (n_1) and film thickness (d_1). One can obtain a formula for the refractive index using Eq. 6 and Eqs. 8a-8b,

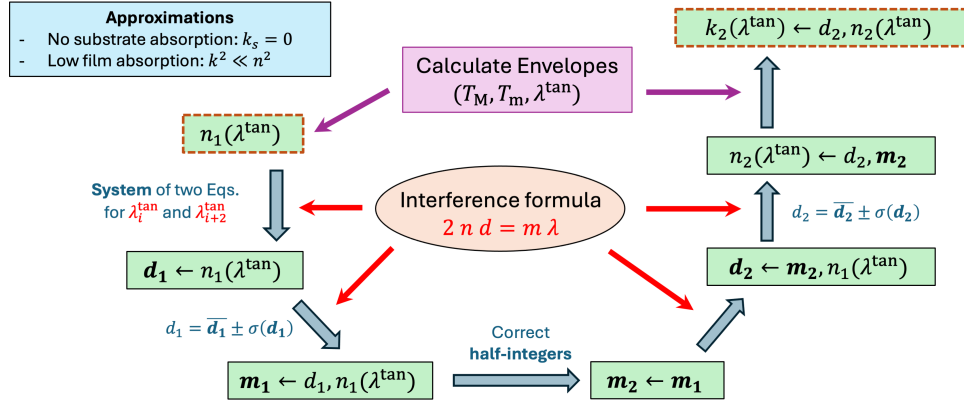


Fig. 4. Summary of the Swanepoel method: the steps are marked in green, starting at the top left. (1) After computing the transmission envelopes, initial estimates of the refractive index n_1 are determined at the tangent wavelengths λ^{tan} . (2) A system of two equations (based on the interference formula) is solved at each pair of adjacent tangents point to estimate the film thickness, resulting in a set of possible thickness $\mathbf{d}_1$. The expected thickness value is calculated as $d_1 = \text{mean}(\mathbf{d}_1) \pm \text{std}(\mathbf{d}_1)$. (3) The interference formula is then applied again to compute the interference orders $\mathbf{m}_1$. (4) These calculated decimal values should theoretically be half-integers, so they are updated to the nearest corrected values $\mathbf{m}_2$. (5) With these corrected interference orders, a more precise thickness estimate $d_2 = \text{mean}(\mathbf{d}_2) \pm \text{std}(\mathbf{d}_2)$ is obtained using the interference formula. (6) This refined thickness allows for updated refractive index values n_2 at the tangent points. (7) Finally, an accurate extinction coefficient k_2 is computed at the tangent points using the precise d_2 , the updated refractive index n_2 , and information from the envelopes.

339 leading to

$$n_1 = \sqrt{N + \sqrt{N^2 - s^2}}, \text{ where} \quad (9)$$

$$N = 2s \frac{T_M - T_m}{T_M T_m} + \frac{n_s^2 + 1}{2}.$$

340 Eq. 9 is then evaluated at each tangent point, yielding the series of values $n_1(\lambda^{\text{tan}})$. Table 2 lists
 341 these computed values $n_1(\lambda^{\text{tan}})$ corresponding to the spectra illustrated in Fig. 1b. Subsequently,
 342 we utilize the fundamental Fabry-Perot interference [71] equation:

$$2n(\lambda)d = m\lambda. \quad (10)$$

343 This well-established relation holds only at the *tangent* points ($\lambda = \lambda^{\text{tan}}$), which explicitly
 344 denote the transition between constructive and destructive interferences, or vice-versa. The
 345 variable m symbolizes the interference order, a number in the set $\mathbb{N}/2 = \{1/2, 1, 3/2, 2, 5/2, \dots\}$
 346 and therefore referred to as a "half-integer." Note that the successive tangent points, arranged
 347 from longer to shorter wavelengths, correspond to consecutive interference orders. For instance,
 348 Table 2 lists the values of m that range from 3.0 to 10.0 for sample #1, with increments of 0.5.

349 Two adjacent upper tangent points (or two adjacent lower points), denoted as λ_i^{tan} and $\lambda_{i+2}^{\text{tan}}$,
 350 have orders of interference m and $m + 1$, respectively. Therefore, we can define the following
 351 system of equations:

$$\begin{cases} 2n_1(\lambda_i^{\text{tan}})d_1 = m\lambda_i^{\text{tan}} \\ 2n_1(\lambda_{i+2}^{\text{tan}})d_1 = (m + 1)\lambda_{i+2}^{\text{tan}} \end{cases} \quad (11)$$

352 Knowing now λ_i^{tan} and $n_1(\lambda_i^{\text{tan}})$ for each tangent point i , we can solve Eq. 11 for the unknown
 353 variable d_1 . The equation can be solved to find the d_1 values for the different tangent points,
 354 except for the two greater ones (as the system needs the points i and $i + 2$). The set of values $\mathbf{d}_1$
 355 represents the thickness estimations using data from the multiple tangent points (see Table 2).
 356 Ideally, each of these d_1 values should be identical. In practice, the thickness is approximated as
 357 $d_1 = \text{mean}(\mathbf{d}_1) \pm \text{std}(\mathbf{d}_1)$.

358 Sometimes, it is advisable to exclude the elements of $\mathbf{d}_1$ corresponding to the shorter
 359 wavelengths if they clearly differ from the the mean value, as they are often not very consistent
 360 with the other values (see the marked numbers on the Table 2). This discrepancy arises when
 361 there exists a strong absorption at shorter wavelengths, as the Swanepoel approximation ($n \gg k$)
 362 becomes less accurate.

363 *Refining the values of n_2 and d_2*

364 The previous estimates are highly sensitive to noise from the experimental transmission measure-
 365 ments and errors in the two corresponding envelopes. Therefore, it is important to go through a
 366 second refinement step to find more suitable values of n_2 and d_2 . First, note that we can now
 367 calculate the “inexact” half-integers (denoted by $\mathbf{m}_1$) by inserting the predicted rough values
 368 $n_1(\lambda^{\text{tan}})$ and d_1 in Eq. 10, yielding $\mathbf{m}_1 = 2n_1(\lambda^{\text{tan}})d_1/\lambda^{\text{tan}}$. The set of approximated values $\mathbf{m}_1$
 369 are shown in the 6th column of Table 2.

370 We know that $\mathbf{m}_1$ should theoretically be half-integers, so we can improve the found values.
 371 Indeed, one will now search for the sequence of consecutive half-integers $\mathbf{m}_2$ that best match the
 372 approximated data $\mathbf{m}_1$. This can be done automatically by solving a fitting problem using the
 373 direct search method, a convenient global optimizer for this simple low-dimensional problem.
 374 The correct values $\mathbf{m}_2$ are shown in the column 7th of Table 2.

375 Setting now $n_1(\lambda^{\text{tan}})$ and the *exact* values of $\mathbf{m}_2$ into Eq. 10, we can determine a new array
 376 $\mathbf{d}_2$ with more accurate film-thickness estimates: $\mathbf{d}_2 = \mathbf{m}_2\lambda^{\text{tan}}/2n_1(\lambda^{\text{tan}})$. The corrected film
 377 thickness is then computed as $d_2 = \text{mean}(\mathbf{d}_2) \pm \text{std}(\mathbf{d}_2)$. These values are shown in the 8th
 378 column of Table 2. In the two example shown in the table, one can see noticeable improvements
 379 from d_1 to d_2 , reducing the uncertainty of the thickness value by an order of magnitude.

380 Finally, one can employ the interference formula once again to compute the corrected refractive
 381 index $n_2(\lambda^{\text{tan}})$. Note that the known values that we introduce in the interference formula are
 382 the exact set of values $\mathbf{m}_2$ and the highly accurate thickness d_2 . In particular, we now compute
 383 $n_2(\lambda^{\text{tan}}) = \mathbf{m}_2\lambda^{\text{tan}}/2d_2$.

384 *Finding k_2*

385 With the refined values of the refractive index $n_2(\lambda^{\text{tan}})$ and thickness d_2 , we now aim to find
 386 precise values of the extinction coefficient $k_2(\lambda^{\text{tan}})$ at each tangent point. Observe that since
 387 the extinction coefficient k , the absorption coefficient α , and the variable x are directly related
 388 through Eqs. 2a–2b, it is sufficient to estimate any one of these quantities. We will then analyze x .

389 The variables (A, B, C, D) from Eq. 7 depend only on n and d , and can now be accurately
 390 calculated using the refined values $n_2(\lambda^{\text{tan}})$ and d_2 . Considering that the envelopes T_M and T_m
 391 were (somehow) previously calculated, we can now solve either Eqs. 8a or 8b for $x_2(\lambda^{\text{tan}})$ at
 392 each wavelength λ^{tan} . It is important to note that these equations are quadratic, resulting in two
 393 possible ambiguous results for x_2 . However, it must be remarked again that the parameter x_2
 394 represents a fraction of transmitted intensity: the beam intensity transmitted in a single pass
 395 through the thin film, neglecting the multiple inter-reflections in the film and the substrate. Of
 396 course, such quantity must lie in the range from 0 and 1, and we can then select the unique
 397 physically meaningful solution within this range, out of the two possible mathematical results.

Table 2. Results of the Swanepoel method applied to the transmission spectra of Sample #1 and Sample #2. The estimated thicknesses are provided along with their standard deviations and relative errors compared to the thicknesses obtained from the inverse synthesis method. For Sample #1, $d_1 = 1099.32 \pm 35.77$ nm (relative error = 3.25%) and $d_2 = 1110.18 \pm 7.22$ nm (relative error = 0.65%). For Sample #2, $d_1 = 1167.28 \pm 62.92$ nm (relative error = 5.39%) and $d_2 = 1163.88 \pm 10.52$ nm (relative error = 0.90%). The last two data points in each sample are crossed out due to unreliable calculations at shorter wavelengths.

Tan (nm)	T_m (%)	T_M (%)	n_1	d_1 (nm)	Half int inexact	Half int exact	d_2 (nm)	n_2	k_2 ($\times 10^3$)	α_2 ($\times 10^3 \text{ cm}^{-1}$)	x_2
Sample #1											
2340.0	44.35	88.46	3.2049	–	3.0113	3.0	1095.19	3.1616	2.9	0.1550	0.9829
2020.0	43.94	88.28	3.1535	–	3.4324	3.5	1120.97	3.1842	4.2	0.2614	0.9714
1776.0	43.35	87.90	3.1818	1185.00	3.9390	4.0	1116.34	3.1995	4.0	0.2836	0.9690
1588.0	42.56	85.61	3.1940	1110.70	4.4222	4.5	1118.68	3.2184	5.6	0.4458	0.9517
1436.0	41.28	82.01	3.2289	1094.23	4.9437	5.0	1111.85	3.2337	7.9	0.6948	0.9258
1316.0	39.72	77.51	3.2443	1101.41	5.4203	5.5	1115.50	3.2598	11.0	1.0545	0.8895
1216.0	37.90	72.17	3.2718	1130.93	5.9157	6.0	1114.98	3.2859	14.5	1.4990	0.8467
1128.0	35.72	65.99	3.3037	1078.69	6.4394	6.5	1109.67	3.3022	18.6	2.0713	0.7946
1056.0	33.39	59.50	3.3333	1073.15	6.9401	7.0	1108.81	3.3292	23.0	2.7408	0.7377
996.0	30.84	52.76	3.3677	1105.09	7.4342	7.5	1109.06	3.3643	28.0	3.5269	0.6760
944.0	27.89	45.57	3.4117	1092.79	7.9461	8.0	1106.78	3.4012	33.9	4.5095	0.6061
896.0	24.33	37.19	3.4421	1086.14	8.4463	8.5	1106.31	3.4301	42.3	5.9310	0.5177
856.0	20.29	29.20	3.5074	1034.42	9.0088	9.0	1098.25	3.4697	52.3	7.6742	0.4266
820.0	15.99	21.16	3.5336	~~1068.99~~	9.4747	9.5	–	–	–	–	–
788.0	11.62	14.25	3.5865	~~1101.34~~	10.0070	10.0	–	–	–	–	–
Sample #2											
2260.0	39.13	89.72	3.4974	–	3.6128	3.5	1130.84	3.3981	1.3	0.0706	0.9918
1992.0	39.12	88.71	3.4246	–	4.0136	4.0	1163.33	3.4230	3.2	0.2050	0.9764
1776.0	39.09	87.20	3.4086	1345.01	4.4806	4.5	1172.33	3.4333	4.3	0.3011	0.9656
1608.0	38.38	85.11	3.4256	1216.15	4.9734	5.0	1173.53	3.4540	5.6	0.4359	0.9505
1472.0	37.27	81.60	3.4566	1165.49	5.4822	5.5	1171.08	3.4780	7.8	0.6642	0.9256
1356.0	35.93	76.99	3.4765	1153.44	5.9854	6.0	1170.13	3.4952	10.8	0.9974	0.8904
1260.0	34.40	71.62	3.5049	1153.61	6.4940	6.5	1168.36	3.5184	14.1	1.4067	0.8490
1180.0	32.75	65.89	3.5296	1170.04	6.9830	7.0	1170.12	3.5485	17.7	1.8860	0.8029
1108.0	30.85	59.89	3.5632	1151.50	7.5077	7.5	1166.08	3.5699	21.6	2.4504	0.7519
1048.0	28.89	53.84	3.5932	1142.88	8.0044	8.0	1166.64	3.6017	25.7	3.0864	0.6982
992.0	26.54	46.93	3.6257	1138.98	8.5326	8.5	1162.82	3.6224	31.1	3.9394	0.6322
948.0	24.05	40.39	3.6679	1135.25	9.0326	9.0	1163.07	3.6653	36.8	4.8776	0.5668
904.0	20.81	32.28	3.6903	1170.02	9.5302	9.5	1163.58	3.6894	45.8	6.3617	0.4769
868.0	17.24	24.95	3.7659	~~1065.04~~	10.1286	10.0	–	–	–	–	–
836.0	13.55	18.09	3.7984	~~1083.89~~	10.6072	10.5	–	–	–	–	–

398 Novel procedure to find the Swanepoel envelopes

399 The previous section explained how to obtain the optical functions using our automated
 400 implementation of the Swanepoel method. Please note that the method did *not* describe how to
 401 find the envelopes from an experimental transmission spectrum or their corresponding tangent
 402 points, but rather assumed that these envelopes were known *a priori*. We now propose our novel
 403 approach to construct the envelopes and solve that initial and particularly challenging problem.

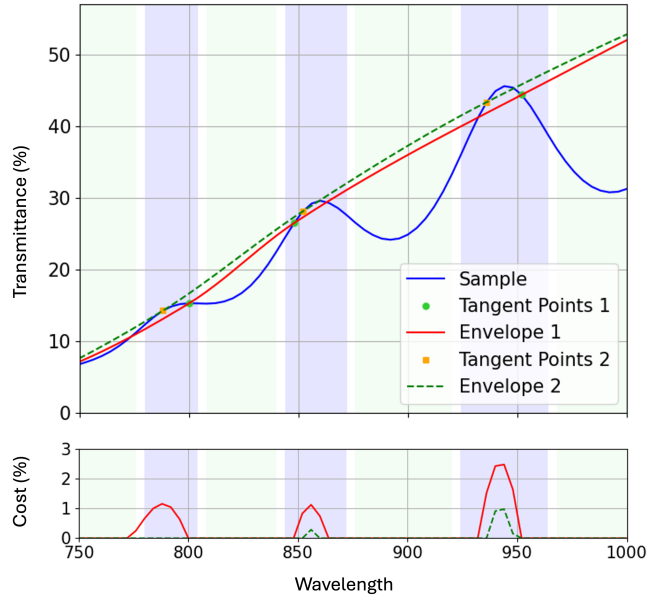


Fig. 5. Graphical illustration of the iterative optimization process used to determine the upper envelope. The algorithm identifies upper tangent points so that the interpolated curve lies entirely above the experimental transmission data, ensuring that each concave region contains a unique tangent point. During the initial iteration (red envelope), the randomly selected tangent points yield a high cost (see bottom panel). In subsequent iterations (green dashed envelope), the cost gradually decreases, allowing the solution to converge to the desired upper envelope.

404 Data treatment and convexity regions

405 Initially, we need to select only the adequate spectral region in which the substrate exhibits
 406 negligible absorption ($k_s \approx 0$), and where the thin-layer sample has *non-zero* transmission
 407 (excluding areas of clear strong absorption), therefore confining our analysis to the spectral region
 408 valid for the Swanepoel method. We then employ a convenient Gaussian filter to reduce noise in
 409 the transmission spectrum of the sample. Finally, we interpolate the transmission curve over
 410 the full wavelength range with *cubic splines*, which ensure the second-order differentiability
 411 of the spectrum. This first step is crucial to find the tangent points with high precision, as the
 412 experimental transmittance measurements might have a relatively low spectral resolution (e.g.,
 413 with measured wavelengths every 10 nm).

414 Following this initial data treatment, we now identify downward concave intervals within the
 415 transmission spectrum by employing the second-order numerical derivatives. The remaining
 416 spectral intervals not identified as concave are consequently categorized as upward convex
 417 intervals. Figure 8 show the convex regions in light green and the concave ones light blue. We

will designate the concave intervals as $[u_t^{\min}, u_t^{\max}]$, for $t \in \{1, \dots, U\}$. Similarly, the convex intervals are denoted as $[v_t^{\min}, v_t^{\max}]$, for $t \in \{1, \dots, V\}$. The resulting intervals must alternate, ensuring the relation $U = V \pm 1$.

Adopting the reasoning presented in [49], we will only incorporate the intervals at the end (either concave or convex) if they possess a local extremum, given that such intervals could potentially encompass a tangent point. In other words, if last interval is severely cropped, not including its minimum or maximum, it should be discarded. For instance, a short interval at the end of both graphs from Fig. 8 appears blank, as it does not contain an extrema. Additionally, the regions in the left-hand side in which $T(\lambda)$ is below a certain numerical threshold (such as 0.5%) are crop out, as no useful information about the tangent point is found in the regions of complete absorption.

In practice, noise in the transmission spectra and small absorption of the substrate typically lead to incorrect interval classification of the convexity. To compensate for this problem, we introduce a “window” variable that establishes the minimum size of the intervals (the highest frequency allowed). Intervals shorter than this window size are considered spurious and are merged with adjacent intervals to form larger, more significant regions. This process effectively filters out inconsistent high-frequency noisy oscillations in the transmission spectrum and its derivatives, ensuring that only meaningful convexity intervals are retained. The selection of this window variable must be customized depending on the unique characteristics of the experimental data and its noise.

Finding the tangent points with an optimization algorithm

After these steps, we formulate a global optimization problem that allows us to simultaneously determine both the tangent points and the envelopes. We incorporate into our model two essential properties of the Swanepoel envelopes, detailed below:

- **Envelopes bound the transmission curve:** The upper envelope consistently lies above the transmission curve, $T^{\text{sim}}(\lambda) \leq T_M^{\text{sim}}(\lambda)$, and the lower envelope lies below it, $T_m^{\text{sim}}(\lambda) \leq T^{\text{sim}}(\lambda)$. Consequently, the transmission curve and its envelopes touch at the tangent points but do not cross each other. This behavior follows from the definition of envelopes (see Eq. 7) and can be readily proved under the reasonable assumption that $n \geq n_s$, which ensures the variable C in Eq. 7 is non-negative.
- **Convexity at tangent points:** Each upper tangent point is located in a concave region of the transmission curve, while each lower tangent point is found within a convex region. To justify this intuitive property, we used symbolic computation software (*Wolfram Alpha Mathematica*) to determine the second derivative of the transmission $T^{\text{sim}}(\lambda)$ at the tangent points². We found that the second derivative is positive at the lower tangent points and negative at the upper ones.

²In spectral regions where the film exhibits medium-to-weak absorption, the optical functions $n(\lambda)$ and $k(\lambda)$ vary only slightly. It is reasonable to consider the variables (A, B, C, D, x) from Eq. 6 as approximately constant around a specific tangent point. Consequently, variations in the transmission spectrum near that point primarily stem from the term $\cos(\varphi)$ in Eq. 6, due to the rapid change of the phase $\varphi = 4\pi nd/\lambda$ with wavelength. This observation allows us to analytically estimate the derivatives of $T^{\text{sim}}(\lambda_{\text{tan}})$.

454 Considering these two reasonable properties for the transmission spectra of thin uniform films³,
 455 we can now define the following minimization problems:

$$\begin{cases} \text{minimize} & C_M(\lambda_1^M, \lambda_2^M, \dots, \lambda_U^M) = \sum_{i=1}^k \text{ReLU} \left[T(\lambda_i) - T_M(\lambda_i; \lambda_1^M, \lambda_2^M, \dots, \lambda_U^M) \right], \\ \text{subject to} & \lambda_t^M \in [u_t^{\min}, u_t^{\max}], \text{ for } t \in \{1, 2, \dots, U\}. \end{cases} \quad (12a)$$

$$\begin{cases} \text{minimize} & C_m(\lambda_1^m, \lambda_2^m, \dots, \lambda_V^m) = \sum_{i=1}^k \text{ReLU} \left[T_m(\lambda_i; \lambda_1^m, \lambda_2^m, \dots, \lambda_V^m) - T(\lambda_i) \right], \\ \text{subject to} & \lambda_t^m \in [v_t^{\min}, v_t^{\max}], \text{ for } t \in \{1, 2, \dots, V\}. \end{cases} \quad (12b)$$

456 The rectified linear unit (ReLU) function, frequently employed in machine learning contexts,
 457 is defined as $\text{ReLU}(x) = x$ if $x > 0$, and $\text{ReLU}(x) = 0$ if $x \leq 0$. This function ensures that the
 458 cost $C_M(\lambda_1^M, \lambda_2^M, \dots, \lambda_U^M)$ penalizes only the instances when the upper envelope is beneath the
 459 transmission spectrum (breaking the first property), while $C_m(\lambda_1^m, \lambda_2^m, \dots, \lambda_V^m)$ penalizes only the
 460 cases where the lower envelope is above the spectrum. Note that the constraint of the optimization
 461 problem guarantees the presence of one (and only one) upper tangent point for each concave
 462 region, and one (and only one) lower tangent point for each convex region, as established in the
 463 second property.

464 The predicted top and bottom envelopes, denoted by $T_M(\cdot)$ and $T_m(\cdot)$, are obtained using cubic
 465 Hermite interpolation [72] on the tangent points. For instance, the upper envelope corresponds
 466 to the interpolation of the points $\{\lambda_t^M, T(\lambda_t^M)\}_t$, for $t \in \{1, 2, \dots, U\}$. Once these points are
 467 interpolated, we can evaluate the upper $T_M(\lambda)$ envelope function at any wavelength λ within the
 468 continuous spectral region, and vice-versa for the lower envelope.

469 The Hermite interpolation provides a piece-wise polynomial approximation of the envelopes,
 470 while maintaining monotonicity within each piece. By utilizing cubic Hermite interpolation, we
 471 not only ensure that the interpolated envelopes pass through the given tangent points but also that
 472 they conform to the specific slopes at those points. This method incorporates both the function
 473 values and their first derivatives, resulting in a piecewise cubic polynomial that is continuous in
 474 both value and slope. The inclusion of derivative information allows the interpolation to capture
 475 the local behavior of the data more accurately, preserving essential features such as peaks and
 476 inflection points. Moreover, cubic Hermite interpolation minimizes oscillations between data
 477 points, a common issue with higher-degree polynomial interpolations that do not consider slope
 478 information. This reduction in unwanted oscillatory behavior leads to a more stable and reliable
 479 approximation of the envelopes.

480 To solve the optimization problems presented in Eqs. 12a-12b, we utilize the Simulated
 481 (Dual) Annealing algorithm [70]. It should be noted that conventional local optimizers (such
 482 as Gradient-Descent, Levenberg-Marquardt, or Nelder-Mead), fail to converge to the correct
 483 solution due to the presence of several local minima. Very significantly, our algorithm converges
 484 in 30-60 seconds on a standard computer, given the simplicity of the cost functions. Figs. 8a-b
 485 show a the results of our envelope-detection algorithm for a simulated sample and a zoom-in of
 486 the strong-absorption region. Figs. 8c-d show the results of our approach for the real samples #1
 487 and #2, respectively.

³Non-uniform films are often modeled using a Taylor first-order approximation with a planar surface exhibiting a certain tilt. A more general expression for the transmission formula in these scenarios is derived in [33]. It should be noted that for films with a very high wedge, $\Delta d > \lambda/(4n)$, the two properties described above do no longer hold. In such cases, the upper and lower envelopes eventually cross over each other, resulting in the upper envelope lying below the spectrum with upper tangent points in convex regions (and vice versa for the lower envelope). Our current study does not apply to this more complex scenario.

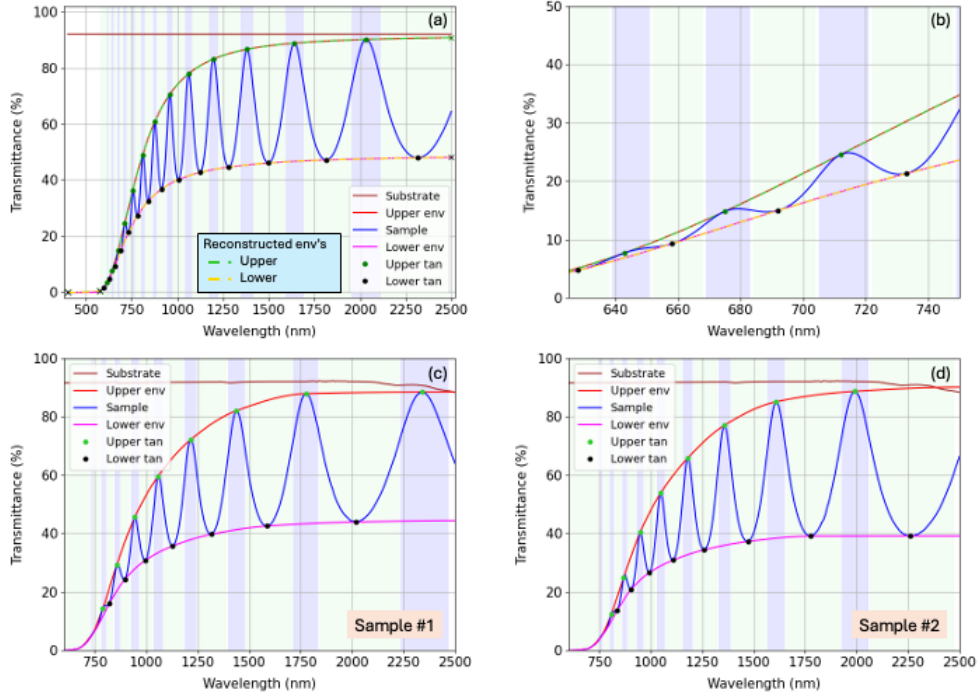


Fig. 6. Envelopes and tangent points determined using our novel optimization procedure. In particular, (a) shows the reconstructions for simulated sample and (b) a magnified view of its strong absorption region, while (c) and (d) show transmittance curves for the real samples #1 and #2, respectively. These results satisfy the two constraints imposed in our optimization problem: first, the upper (lower) envelope consistently lies above (below) the transmittance curve, touching it only at upper (lower) tangent points; second, these tangent points are localized within the light-blue concave (upper) or light-green convex (lower) regions.

488 *Boundary points*

489 Interpolation near the edges of the spectral region of interest (ROI) can be challenging, particularly
 490 at the first and last tangent points. To improve accuracy, we propose extending the envelope
 491 calculation to include boundary points at both ends of the ROI rather than stopping at the first
 492 and last tangent points. This ensures that the first and last tangent points become interior nodes
 493 rather than endpoints, improving the stability of the interpolation. The selection of boundary
 494 points is informed by the film's behavior at both extremes of the spectrum.

495 **First boundary point(s):** At shorter wavelengths, where absorption is strong, the amplitude
 496 of the oscillations decrease, and the upper and lower envelopes converge toward the measured
 497 transmittance $T(\lambda_{\text{init}}) \approx 0$, indicating that the film is essentially opaque (see Fig. 6a below 600
 498 nm). Thus, an additional boundary node $(\lambda_{\text{init}}, T(\lambda_{\text{init}}))$ is placed at the initial wavelength for
 499 both the upper and lower envelopes. In cases where the region of near-complete absorption is not
 500 fully cropped, one can place this boundary node at the earliest wavelength where $T(\lambda_{\text{init}}) \approx 0$
 501 still holds true. One can see these first two added boundary points in Fig. 6a.

502 **Last boundary point:** At longer wavelengths, where absorption weakens and the envelopes
 503 flatten, we approximate the last boundary point $(\lambda_{\text{last}}, y_{\text{last}})$ using a simple parabolic model
 504 based on the *two final tangent points*, denoted (λ_1, y_1) and (λ_2, y_2) . In this ending region, the
 505 tangent points indeed lie very close to the local extrema, making this approximation convenient

506 in practice. Specifically, we assume the mathematical model:

$$y_{\text{last}} = T_0 + \frac{T_1}{\lambda - \lambda_0}, \quad (13)$$

507 Where the amplitude $T_1 \in [0, 1]$ and wavelength λ_0 are determined analytically from the two
 508 last maxima (λ_1, y_1) and (λ_2, y_2) for the upper envelope, or minima for the lower envelope. The
 509 parameter T_0 is fix to the mean substrate absorption T_s in the case of the upper envelope: in
 510 the weak absorption region, the upper envelope naturally converges to the almost flat curve of
 511 the transmittance. In the case of the lower envelope, we calculate the distance between the last
 512 maximum and minimum values, which approximates $T_M^{-1} - T_m^{-1}$ at the end of the spectrum. We
 513 then know that, in the region of weak absorption, the lower envelope must eventually convergent
 514 for longer wavelengths to the value $T_0 = T_s - (T_M^{-1} - T_m^{-1})$.

515 By integrating this physically informed boundary treatment, we ensure a smoother and more
 516 reliable envelope estimation across the entire ROI. Note that alternative boundary conditions may
 517 be employed for other type of spectra, such as those not reaching near-zero transmittance at the
 518 short-wavelength limit, not approaching a medium-to-weak region at the long-wavelength end, or
 519 reaching the completely non-absorption region at the long-wavelength end. Our implementation
 520 allows users to select different boundary models, such as a flat envelope at the long-wavelength
 521 side when complete transparency is reached, exponential and linear fits from the two first or last
 522 tangent points, and even manual selection, for more pathological cases.

523 Other envelope construction techniques

524 We now present an overview of three envelope construction approaches, including (i) the widely
 525 employed McClain iterative algorithm [49], (ii) the practical parabolic or exponential fitting
 526 methods, and the recently devised (iii) deep learning technique [60], all of which will serve as
 527 benchmarks for evaluating our approach in the subsequent section. The implementation of other
 528 methodologies proposed in the literature [53–56], for which no openly available code exists, is
 529 beyond the scope of this study.

530 *McClain algorithm*

531 The most widely employed and established algorithm for envelope construction was developed
 532 by McClain et al. in 1991 [49]. This technique consists of two distinct phases: first estimating
 533 the tangent points and then refining them.

534 In the *first* phase, one identifies the local minima and maxima of the transmission curve,
 535 tentatively assigning them as the lower and upper tangent points. Since not all tangent points
 536 coincide with peaks and valleys, an alternative approach involves selecting the midpoints of the
 537 concave and convex regions. These estimated tangent points are then used to construct the first
 538 approximated lower and upper envelopes via B-spline interpolation. The initial estimation of the
 539 tangent points during the first phase is the most critical part to find accurate envelopes.

540 Observe that the algorithm requires the first and last tangent points, located at the boundaries
 541 of the interval, to coincide with local extrema (i.e., maxima for the upper envelope and minima
 542 for the lower envelope). While this approach helps avoid including invalid or spurious points,
 543 as noted in the seminal reference [49], it also leads to drawbacks. For one, it may produce
 544 larger errors, as evidenced by the substantial shift from the first extremum to the corresponding
 545 tangent point (see Fig. 1d). Moreover, it excludes many potentially useful tangent points in
 546 the shorter-wavelength region where small oscillations often occur without forming clear local
 547 maxima or minima⁴.

⁴In broadband transmission measurements, the spectrum typically transitions from strong absorption near the optical bandgap to moderate or weak absorption further away. Early in the spectrum, small oscillations frequently arise without distinct local extrema. By requiring that the first tangent point be a local extremum, the algorithm effectively discards

548 In the *second* phase, the algorithm iteratively refines the tangent points to improve the accuracy
 549 of the envelopes. Focusing on the upper envelope, the algorithm identifies “incorrect” regions
 550 in which the estimated upper envelope $T_M(\lambda)$ falls below the actual transmission spectrum
 551 $T(\lambda)$. The upper tangent points are then relocated to the midpoints of these incorrect regions,
 552 as done in the bisection method. A new upper envelope is recalculated based on the updated
 553 tangent points. This iterative process is repeated until convergence (or up to a maximum of
 554 20 times), progressively reducing the size of the incorrect regions at each step. Note that the
 555 same refinement procedure is applied to the lower tangent points and envelope. In this case, the
 556 incorrect regions are those where the estimated lower envelope $T_m(\lambda)$ lies above the transmission
 557 spectrum $T(\lambda)$.

558 *Parabolic or exponential fitting*

559 Another prevalent technique involves the direct fitting of local maxima (or minima) using either
 560 parabolic or exponential curves to construct the upper (or lower) envelopes. The envelopes then
 561 follow one of these mathematical expressions:

$$f^{\text{para}}(\lambda; T_0, T_1, T_2, \Lambda_1, \Lambda_2) = T_0 + \frac{10^2 \cdot T_1}{\lambda - \Lambda_1} + \frac{10^5 \cdot T_2}{(\lambda - \Lambda_2)^2} \quad (14a)$$

$$f^{\text{exp}}(\lambda; T_0, T_1, T_2, \Lambda_1, \Lambda_2) = T_0 + T_1 \cdot e^{-\lambda/\Lambda_1} + T_2 \cdot e^{-\lambda/\Lambda_2} \quad (14b)$$

562 The optimal parameters $(T_0, T_1, T_2, \Lambda_1, \Lambda_2)$ can be obtained by solving a nonlinear least-square
 563 fitting problem. Although generally less precise than McClain algorithm, it is crucial to point out
 564 that this fitting approach is notably beneficial for transmission spectra that exhibit a restricted
 565 number of oscillations and tangent points, a condition often encountered with ultra-thin films.
 566 The piece-wise interpolations used in both the McClain algorithm and our newly proposed
 567 methods typically require at least four tangent points for a reliable estimation of each envelope.

568 The fitting method has also proved valid [57] for crystalline film materials, where the materials
 569 present a distinct absorption band and are almost transparent beyond the absorption region. These
 570 materials have an almost nonexistent Urbach tail, given their low level of molecular disorder.
 571 In this cases, the subsequent very flat envelope curves can be conveniently modeled by Eqs.
 572 14a-14b, independently of the amount of present oscillations in the transmission spectrum.

573 Our method introduces the artificial boundary points at the ends of the spectral range using
 574 a similar approach, but applying first-order parabolic or exponential functions rather than a
 575 second-order ones. This adjustment ensures that the fitting procedure is well-defined and depends
 576 only on the final two nodes, enabling a direct analytical solution.

577 *Deep learning approach*

578 While both McClain and the curve-fitting algorithms offer reasonable outcomes in practice and
 579 converge to an envelope of an oscillating function, they do not necessarily converge to the exact
 580 expression of the Swanepoel envelopes, as defined in Eqs. 8. To overcome this issue, our group
 581 developed a deep learning (DL) approach [60] that calculates the envelopes in alignment with the
 582 Swanepoel theoretical expressions. In particular, we created a dataset of 100,000 input-output
 583 pairs $\{T(\lambda), T_M(\lambda)\}$ for training using the exact Eqs. 6-8a. A supervised Convolutional Neural
 584 Networks (CNNs) model was trained with this dataset to predict the upper and lower envelopes
 585 from a transmission spectrum in real-time. While this DL model does not have limitations on the
 586 number of tangent points, it is susceptible to noise and artifacts from real-world transmission
 587 measurements. This is caused because the distribution of the simulated data differs significantly,

these non-extremal oscillations, undermining the intended benefit of using the midpoints of concave/convex intervals instead of the peaks/valleys as initial tangent point candidates.

588 which is a known issue for DL approaches used in inverse problems like image restoration or
589 super-resolution [73–76].

590 The noise in real measures strongly depends on the instrumentation and the conditions of the
591 particular experiment. For instance, one potential sources of deviance between the simulated and
592 real spectra is the photodetector noise, which can be responsible up to the 0.2% transmittance
593 error. Second, the effect of the realistic limited coherent length of the beam in the thin film,
594 which affects the peaks and valleys. Third, the increase of coherent length with the wavelength,
595 which may eventually lead to the high frequency noise due to the undesired thick-substrate
596 interferences. Fourth, the change in the emitting source for UV versus VIS-NIR, which may
597 produces a significant jump in the transmittance. Fifth, the substrate absorption of at particular
598 wavelengths, and the absorption of air components if the experiment is not carefully performed
599 in a vacuum. Observe that modeling these noise sources in general is challenging and not yet
600 fully addressed in the current literature. Incorporating a comprehensive theoretical noise model
601 could enhance the current DL approach by providing deeper insights and improving its overall
602 performance with real data.

603 Validation and comparison

604 We began by validating our envelope construction procedure using 50 computer-generated
605 transmission spectra, each accompanied by a known theoretical envelope. In particular, we
606 generated 50 random set of parameters ($d, E_0, E_d, \alpha_0, E_u$) within the bounds specified in Table 1.
607 These data were then employed in Eq. 6 to produce the transmittance, and Eqs. 8a-8b for their
608 corresponding envelopes. The substrate transmittance is assumed constant, with the typical value
609 $T_s = 92\%$.

Method	Upper env.	Lower env.	Upper tan	Lower tan
McClain	0.202 ± 0.129	0.090 ± 0.040	2.59 ± 1.75	2.48 ± 1.45
Ours	0.080 ± 0.078	0.043 ± 0.034	0.27 ± 0.33	0.55 ± 0.72

Table 3. Comparing our proposed method with respect to the standard McClain algorithm within the same spectral region (between the first and last local extrema).

610 Accurate envelope determination relies on the inclusion of boundary points. For the first
611 boundary point, corresponding to a regime of nearly complete absorption ($T \approx 0$), the estimation
612 is straightforward in our simulated samples, as the chosen spectral range encompasses the strongly
613 absorbing region near the band gap. In contrast, determining the last boundary point is a more
614 challenging task. Comparison of our default parabolic-fitting model with the known ground-truth
615 last boundary point resulted in a transmittance error of $0.143 \pm 0.214\%$ for the upper boundary
616 point and $0.142 \pm 0.125\%$ for the lower boundary point.

617 Applying our envelope detection procedure to the simulated spectra yielded an RMSE of
618 $0.098 \pm 0.084\%$ for the upper envelope and $0.058 \pm 0.045\%$ for the lower envelope. The slightly
619 higher RMSE for the upper envelope is attributed to its intrinsically larger values. Notably, *all*
620 tangent points were correctly identified, with an average absolute error of 1.06 ± 0.95 nm for
621 the upper tangent points and 2.99 ± 2.62 nm for the lower tangent points. Table 3 compares
622 our method performance to that of the standard McClain algorithm. Because McClain method
623 identifies only tangent points associated with local extrema, the spectral range in which it
624 computes the envelopes is considerably shorter than the full region of interest. To ensure a fair
625 comparison, we restrict both methods to the same shorter spectral region. Our method achieves
626 less than half the RMSE for the envelopes and an absolute error on tangent point location that is
627 more than an order of magnitude smaller.

For a further comparison with curve-fitting approaches, we restrict analysis to spectra with fewer than five tangent points associated with extrema and generate 50 computer-simulated spectra by varying the sample thickness from 200 to 500 nm only, considering ultra-thin film samples. The reported RMSE for the envelopes is computed between the first and last identified tangent points. Under these conditions, the exponential fit yields an error of 2.11% for the upper envelope and 0.31% for the lower envelope, whereas the parabolic fit produces errors of 1.19% (upper) and 0.42% (lower). Because the tangent points in these fits are directly (and somewhat imprecisely) tied to local extrema, their errors increase considerably: 6.10 nm for the exponential fit and 7.66 nm for the parabolic fit. As noted previously, the DL algorithm achieves very low errors (0.14% for the upper and 0.05% for the lower envelopes) over the entire spectral range, but it remains incompatible with realistic noisy data and does not directly provide the locations of the tangent points.

It is important to recognize that the exact optical properties and ground-truth envelopes are obviously unavailable for the case of real spectra, unlike the case with simulated data. To address this limitation, we leverage the results of inverse synthesis as a benchmark for assessing the optical characterization analysis performed by `swanpy`. This comparison should thus be viewed as a *consistency check* rather than a strict accuracy evaluation.

1. First, Fig.7 shows good agreement between the optical functions n and k extracted via inverse synthesis (continuous curves) and those evaluated at specific tangent points by our improved Swanepoel method.
2. Second, the Swanepoel method demonstrates reliable accuracy for determining film thickness. As shown in Table 2, sample #1 exhibits a relative thickness error of 0.65%, while sample #2 has an error of 0.90%. Notably, the thicknesses from inverse synthesis ($d = 1117$ nm for sample #1 and $d = 1160$ nm for sample #2) both lie within the corresponding Swanepoel confidence intervals ($d = 1110 \pm 7$ nm for sample #1 and $d = 1163 \pm 11$ nm for sample #2).
3. Third, an indirect but informative way to validate envelope detection in real measurements is to analyze the interference orders from Table 2. We find that the computed orders m lie very close to half-integer values (columns 6 and 7), indicating an accurate determination of tangent points and envelopes. When misidentified tangent points do occur, their associated interference orders tend to align with other half-integer values rather than the expected one.

This consistency across multiple metrics supports the robustness of our approach for real experimental data.

Conclusions

In this work, we present a novel algorithm for Swanepoel envelopes construction, an essential aspect in the optical characterization of thin films. Our approach integrates the physical properties of the Swanepoel envelopes into a global optimization problem. After evaluation with fifty computer-generated spectra, our algorithm demonstrated an RMSE below 0.01% for the upper envelope and 0.06% for the lower envelope, significantly surpassing the performance of existing state-of-the-art methods. We also successfully applied our approach to characterize two real samples of amorphous silicon.

Additionally, we integrated our envelope construction algorithm with our automated implementation of the Swanepoel method in an open-source Python package, `swanpy`. Given its noise robustness, high accuracy, and speed, our program emerges as a valuable tool for the optical characterization of thin solid films. Future research could potentially explore the applicability of our approach in more complex scenarios, such as non-uniform films, multi-layer samples, or absorbent substrates.

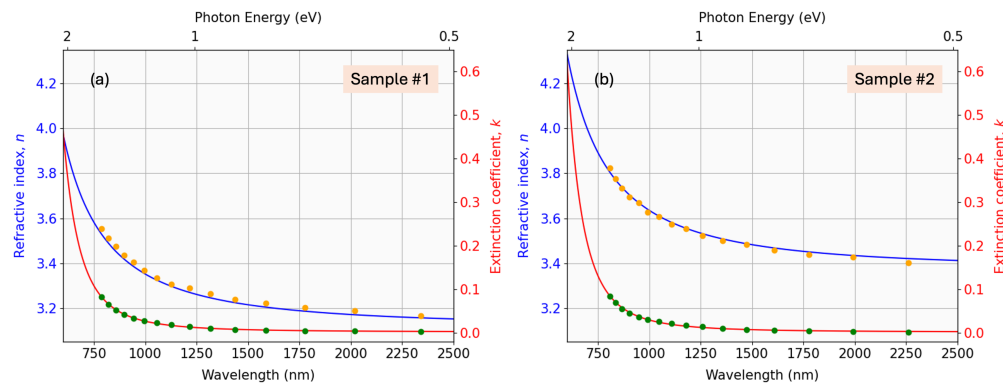


Fig. 7. Refractive index and extinction coefficient for *a*-Si samples #1 and #2, found with the inverse synthesis approach (solid lines) and with our proposed improved Swanepoel method (circles).

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