Procedure to convert optical-constant models into analytic

JUAN I. LARRUQUERT[1,*], LUIS V. RODRÍGUEZ-DE MARCOS [1,2]

[1]*GOLD-IO-CSIC Instituto de Óptica-Consejo Superior de Investigaciones Científicas, Serrano 144, 28006 Madrid, Spain*
[2]*Singapore Synchrotron Light Source, National University of Singapore, 5 Research Link, Singapore 117603*
* *j.larruquert@csic.es* Phone: 34-915616800+940367
2: slslvrd@nus.edu.sg

Abstract: Several common optical-constant models do not satisfy a necessary requirement: they are not analytic (in the sense of holomorphic). This includes models defined with a piecewise function like Tauc-Lorentz, Cody-Lorentz (CL), and Campi-Coriasso, and models with poles in the upper complex half plane. The consequence of this is an intrinsic inaccuracy. Sellmeier model, even though analytic, involves mostly unnatural divergences. A procedure is presented that turns non-analytic optical models into analytic by using the original model as a weight function in an integral over the spectrum using a small broadening parameter. Specific equations are obtained for the weight function being either the dispersion or the absorption part of the optical constants of the non-analytic model. The resulting optical-constant model can be differentiated to any order. The procedure is applied to turn analytic CL model and to remove the divergences from Sellmeier model. The analyticized CL model is applied to fit boron film optical constants.

Keywords: Optical constants; Optical models; Optical properties of semiconductors; Optical properties of thin films; Optical materials

1. Introduction

The optical properties of various groups of materials in nature have common features that allow the use of simple models to describe them in certain spectral ranges. Models depend on few parameters to be determined for each specific material. Thus the refractive index of the dielectric materials can be described with simple models, such as Cauchy and Sellmeier models, which are commonly used in the visible and adjacent ranges. Another group of materials with various available optical-constant models is semiconductors [1].

Models describing the optical constants of materials, either n and k or ε_1 and ε_2, should preserve fundamental properties such as causality. Causality results in that optical constants must be described with a function that is analytic in the upper complex half plane [2]; here analytic will be used in the sense of holomorphic. An example of a model satisfying this requirement is the Lorentz oscillator. However, most other commonly-used models do not satisfy the analyticity requirement. This includes popular models like Forouhi and Bloomer [3], Tauc-Lorentz [4], Cody-Lorentz (CL) [5,6], and others. The lack of analyticity of a function implies that it does not qualify to represent the optical constants of a real material, so that it involves an intrinsic inaccuracy.

The analyticity requirement appears even more obvious when derivatives of the optical constants need to be calculated. The evaluation of optical-constant derivatives up to third order is sometimes required [7], for which analyticity is an essential condition to avoid discontinuities and/or nonsense functionalities.

In fact, the analyticity requirement is not rigorously necessary in the real axis, i.e., for real values of wavelengths or photon energies, but it is necessary in the upper complex half plane up to the limit when the imaginary part of wavelength/photon energy tends to zero [8]. For instance, even though Sellmeier model still satisfies the requirement of analyticity, it involves divergences in the real axis. Such divergences are not found in the typical materials that are described with this model, so that removing these divergences is desirable, in spite of the model not strictly violating the analyticity requirement.

The present paper proposes a procedure to transform non-analytic models into analytic. It can also be used to remove unnatural divergences. It consists of using the existing function of one of the optical constants, either n, k, ε_1, or ε_2, as a weight function in an integral over photon energy. The present procedure is applied to Sellmeier model, which is turned into Lorentz oscillators, and to CL model, which is turned analytic.

The procedure is suitable to apply on models that, even though successful at describing the optical constants of some materials in a certain spectral range, are described with non-analytic functions and hence do not satisfy a necessary requirement. A big group of non-analytic optical-constant models includes those defined with piecewise functions; they are not analytic since they cannot be assigned a unique complex

analytic continuation function. This is the case for models with a functionality change at a gap energy, such as Forouhi and Bloomer [3], Tauc-Lorentz [4], and CL [5,6]. It also occurs with models describing materials that, instead of Tauc's parabolic bands, they follow cubic [9] or even linear laws (amorphous Se) [10]. All these models switch either to no absorption or to an Urbach tail below the gap, which renders the model non-analytic due to the function switch. The same can be said of Campi-Coriasso model [11]. The model derived by Franta *et al.* includes several terms involving piecewise functions [12]. Other models not satisfying the analyticity requirement are those that involve poles in the upper complex half plane, divergences at large complex energies in the same half plane or models that fail at the parity requirement [7,13,14]. The above models are candidates to turn analytic with the present procedure. The lack of analyticity cannot be solved with the present procedure on some models like Forouhi and Bloomer because of a further shortcoming of such model due to the insufficient convergence at high energies in the real axis.

The paper is organized as follows. In section 2 we derive the mechanism to turn one optical constant function into a weight function of an analytic model. In section 3 the mechanism is applied to Sellmeier model and to CL model; the analyticized CL model is applied to fit boron film optical constants.

2. Using a single optical constant to generate an analytic complex optical function

Let us start by expressing the complex dielectric function $\tilde{\varepsilon} = \varepsilon_1 + i\varepsilon_2$ (the procedure is extended in Appendix to $\tilde{N} = n + ik$) as an integral of one of its parts over the spectrum. For this we will use the Sokhotski–Plemelj theorem [15]:

$$\lim_{\delta\to 0^+} \int_{x_1}^{x_2} \frac{f(x)}{x - i\delta} dx = P\int_{x_1}^{x_2} \frac{f(x)}{x} dx + i\pi f(0) \tag{1}$$

where P stands for the Cauchy principal value. In general *f* is a complex function that is continuous on the real axis, and it is satisfied that $x_1<0<x_2$. The theorem is applied here to a real function as a particular case of a complex function. The proof of Eq. (1) consists in multiplying numerator and denominator in the left term by the complex conjugate of the denominator; then we immediately get that the real (imaginary) part of the fraction equals the first (second) term of the right hand side of Eq. (1), where we use the definition of the Dirac delta function in the imaginary part.

We start applying the theorem to the imaginary part of the dielectric function:

$$\begin{aligned} &\lim_{\delta\to 0^+} \int_{-\infty}^{\infty} \frac{\varepsilon_2(E')}{E' - E - i\delta} dE' = P\int_{-\infty}^{\infty} \frac{\varepsilon_2(E')}{E' - E} dE' + i\pi\varepsilon_2(E) \\ &= \pi\left[\varepsilon_1(E) - 1\right] + i\pi\varepsilon_2(E) = \pi\left[\tilde{\varepsilon}(E) - 1\right] \end{aligned} \tag{2}$$

where Kramers-Kronig (KK) dispersion relations have been applied to obtain ε_1-1 through integration of ε_2 over the spectrum. Going from Eq. (1) to (2) is straightforward with a simple variable change and by taking the integration limits to infinity. The idea behind Eq. (2) is to express the full complex dielectric function through integration of only one if its parts (the real or the imaginary part). In fact, a similar development can be made using ε_1-1 in Eq. (1) giving rise to the two following equations:

$$\lim_{\delta\to 0^+} \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\varepsilon_2(E')}{E' - E - i\delta} dE' = \tilde{\varepsilon}(E) - 1 \tag{3a}$$

$$\lim_{\delta\to 0^+} \frac{-i}{\pi} \int_{-\infty}^{\infty} \frac{\varepsilon_1(E') - 1}{E' - E - i\delta} dE' = \tilde{\varepsilon}(E) - 1 \tag{3b}$$

We will use the above expressions to develop a procedure to turn non-analytic optical models into analytic. To modify an optical constant model, we will work not in the limit of null δ but with a finite, although small, value. For this, we convolve the two sides of Eqs. (3a) and (3b) with a Lorentzian function of semi-width *a*:

$$\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\varepsilon_2(E')}{E'-E-ia}dE'=\int_{-\infty}^{\infty}\left[\tilde{\varepsilon}(E')-1\right]\frac{a/\pi}{a^2+(E'-E)^2}dE'=\tilde{\varepsilon}_A(E)-1 \quad \text{(dielectrics) (4a)}$$

$$-\frac{i}{\pi}\int_{-\infty}^{\infty}\frac{\varepsilon_1(E')-1}{E'-E-ia}dE'=\int_{-\infty}^{\infty}\left[\tilde{\varepsilon}(E')-1\right]\frac{a/\pi}{a^2+(E'-E)^2}dE'=\tilde{\varepsilon}_A(E)-1 \quad \text{(dielectrics) (4b)}$$

In the derivation of Eqs. (4a) and (4b) we use that the convolution of two Lorentzian functions is a Lorentzian function. Eqs. (4a) and (4b) express that if we allow for some broadening a (a>0, where a is a real number) in the integration of the specific part (real or imaginary) of the dielectric function [left term in Eqs. (4a) and (4b)], we get to a convolution of the complex dielectric function with a Lorentzian function [middle term of Eq. (4)], i.e., we are averaging the dielectric function with a larger weight in the E±a range, although the integral extends to the whole spectrum. The integration of the left term, which involves poles only in the lower half plane if ε_1 or ε_2 in the integrand are finite, results in a dielectric function $\tilde{\varepsilon}_A(E)$ [right term in Eq. (4)] that is analytic both in the upper half plane and on the real axis. Eq. (4) is valid for dielectrics. With a dielectric material it is meant here that its optical constants do not have a pole at E=0; the case of conductors is addressed below.

Eq. (4) expresses that an analytic dielectric function $\tilde{\varepsilon}_A(E)$ is obtained by a continuous superposition of 1/(E'-E-ia) functions using either the real or the imaginary part of the dielectric function as the weight function. Hence 1/(E'-E-ia) functions are a natural set of functions of this procedure to develop the optical constants as a superposition of them.

The dielectric function of conductors involves a pole at E=0, which requires a modification of Eq. (4). We can adapt the present formalism to metals with a pole at zero energy that conforms to the one of a Drude model (that will be referred to as Drude-type metals) by broadening just the part of the optical function that does not contain the pole. So we subtract the term $i\sigma_{DC}h/2\pi\varepsilon_0 E$ from the complex dielectric function:

$$\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\varepsilon_2(E')-\frac{\sigma_{DC}h}{2\pi\varepsilon_0 E'}}{E'-E-ia}dE'=\int_{-\infty}^{\infty}\left[\tilde{\varepsilon}(E')-1-\frac{i\sigma_{DC}h}{2\pi\varepsilon_0 E'}\right]\frac{a/\pi}{a^2+(E'-E)^2}dE'=\tilde{\varepsilon}_A(E)-1-\frac{i\sigma_{DC}h}{2\pi\varepsilon_0 E} \quad \text{(Drude-type metals) (5a)}$$

$$-\frac{i}{\pi}\int_{-\infty}^{\infty}\frac{\varepsilon_1(E')-1}{E'-E-ia}dE'=\int_{-\infty}^{\infty}\left[\tilde{\varepsilon}(E')-1-\frac{i\sigma_{DC}h}{2\pi\varepsilon_0 E'}\right]\frac{a/\pi}{a^2+(E'-E)^2}dE'=\tilde{\varepsilon}_A(E)-1-\frac{i\sigma_{DC}h}{2\pi\varepsilon_0 E} \quad \text{(Drude-type metals) (5b)}$$

The broadened analytic function with the Drude-type pole at E=0 is given by $\tilde{\varepsilon}_A(E)-1$. The resulting model will be analytic, with the familiar pole at E=0 of Drude metals.

The name "Drude-type metals" means here that the model is applied to metals with a pole at E=0 with the same functionality that in the Drude model, and it does not mean that we are modifying Drude model. The subtracted term involves the material DC conductivity σ_{DC} (in the International System of Units), along with Planck's constant h and the permittivity of vacuum ε_0.

The above equations can be also presented in other useful forms; one form is obtained by replacing the dielectric function with the refractive index. Other forms use the parity of the optical constants, or modify the equations to obtain a Lorentz oscillator-type expression. These equations are developed in the appendix and are summarized in table A.1.

Eqs. (4) or (5), along with those given in Table A.1, can be used to obtain an analytic optical function through Lorentzian broadening of an optical function that is not analytic. As the starting function we can use either the real or the imaginary part of the dielectric function or refractive index. Analyticity with the application of the aforementioned equations is obtained through integration with a broadening parameter a; the poles after integration are located in the lower complex half plane, what turns the function analytic in the upper plane.

Let us see how to apply the above equations to turn analytic some optical-constant model lacking analyticity, such as any of the ones mentioned in section 1. In order to turn it into analytic we take the model for one optical constant, either ε_1 or ε_2 (but also n or k, with equations given in Table A.1), and use it as a real (i.e., non-complex) weight function in the left term of Eq. (4a) or (4b) [other possible equations are (A.1) to (A.2); (A.4) to (A.6) are used when the weight function is the refractive index.] The result can be seen in the

middle term of Eq. (4): a Lorentzian broadening of the complex dielectric function; the extent of the broadening is given by parameter *a*, i.e., the largest contribution comes from the $E\pm a$ range (middle term of all equations in Table A.1). For a specific case, *a* can be made as small as necessary (but not zero), so that this broadening effect may often be made negligible. If we took $a=0$, analyticity would be lost again and we would return to the original non-analytic function.

The obtained optical function must satisfy the rest of mathematical requests. Other than continuous, the weight function needs to have a fast enough decay at infinite photon energy, which results from the function being square-integrable. Finally, the correct parity for the optical-constant function, i. e., $\tilde{\varepsilon}\left(-E^*\right)=\tilde{\varepsilon}^*\left(E\right)$, is provided by the $1/(E'-E-ia)$ functions along with the required odd (even) functionality for the weight function ε_2 (ε_1). * stands for the complex conjugate. When the weight function is given only for positive energies, the function is extended to negative energies by imposing the required parity.

The integral (convolution) of the weight function with $1/(E'-E-ia)$ functions to generate the analytic model can be interpreted as a continuous linear superposition of infinitesimal weight of such functions with their pole in the lower complex half plane, so that no pole is present in the upper complex plane and analyticity is assured as long as the weight function is square-integrable.

The present procedure to turn non-analytic models into analytic has been successfully applied to the Tauc-Lorentz model [16], but the formalism to analyticize the model has never been reported until now and it is presented here.

The candidate models that could be improved with the present procedure are:

- Models described by piecewise functions. Such models are non-analytic because they have at least two functionalities, and the present procedure turns them into analytic. Various examples of these models are given in Section 1.

- Models with 1) poles in the upper complex half plane and/or 2) with divergences at infinite energies in this same half plane and/or 3) failing the parity requirement. The method can be applied assuming that the model has no poles in the real axis and it converges fast enough at large real energies.

- Models with simple unnatural poles in the real axis, such as Sellmeier model. Strictly speaking, they are analytic in spite of the divergence at the poles. The procedure enables removing the divergences.

Regarding the last group, Drude model has a natural pole at E=0 but this does not violate the analyticity requirement.

Eqs. (4), (5), and others given in Table A.1 are proposed to apply on optical-constant models to solve their lack of analyticity. The development of optical constants in an integral of functions with Lorentz or Gaussian broadening has been proposed as methods to fit experimental data [17,18,19]. An essential difference with the present procedure is that the latter is developed to apply to a parametric optical-constant model and it attempts to cover a broad spectrum, whereas the previously reported research was devoted to directly fit experimental data through integration with Lorentz or Gaussian functions and to do it in a small fraction of the spectrum that contains a specific feature of the material.

An interesting procedure was developed by Adachi [1,20] to obtain a simplified optical-constant model for the interband transitions of semiconductors. Adachi's procedure starts with a piecewise function to describe ε_2 in some spectral range from which ε_1 is calculated with KK analysis. Adachi's procedure continues with replacing the real-valued photon energy variable of ε_1 with a complex variable given by $E+i\Gamma$, by adding, in a phenomenological manner, a damping effect through an imaginary parameter $i\Gamma$. This avoids the divergences of the obtained ε_1 function present at some real-valued energies. The resulting function is taken as the full complex dielectric function. The procedure has proved to fit well several materials [1,20]. Even though there might be some similarity with the present procedure, the two procedures involve a different philosophy. Adachi's procedure relies on Γ not only to remove the divergences of ε_1 but also to fully generate ε_2, which can be very different from the starting function, so that Γ must be as large as necessary for this second task. In the present procedure, parameter *a* can be made as small as necessary, regardless how large ε_2 is, so that the final analytic function ε_2 mimics the starting function as much as possible.

3. Application on specific models

3.1 Sellmeier model

Sellmeier model, although still satisfying the analyticity requirement as mentioned in the introduction, involves unnatural divergences, which can be removed with the application of the procedure developed in Section 2. Sellmeier model involves one or several simple poles on the real axis, i.e., the usual photon energy

variable, but these poles are still compatible with the complex continuation function to be analytic in the upper plane. However, the divergence at each resonance energy in Sellmeier model is not observed in typical materials that are described with this model, such as oxides in the visible and UV. The application of the present procedure will turn Sellmeier model into Lorentz oscillators. The connection between Sellmeier model and Lorentz oscillators had already been observed in the literature [21] and such connection may be considered intuitive. In spite of this, it is developed here to exemplify a simple application of the procedure presented in Section 2.

Sellmeier [22] provided an improved model compared to Cauchy's one by obtaining an equation that was successful to describe anomalous dispersion:

$$n^2(E) = 1 + \sum_j \frac{B_j}{E_j^2 - E^2} \tag{6}$$

In Sellmeier's expression, E_j are resonance energies that must be outside the range described by the model; moreover, absorption must be small in the modelled range, and hence $n^2 \approx \varepsilon_1$. E_j and B_j are free parameters to fit the experimental data. When we get close to a resonance, the model goes to infinity, which can be considered unphysical, at least for the typical materials that are described with this model.

The mechanism derived in Section 2 is used here to remove the divergences. By using Sellmeier formula in ε_1 as a weight function in Eq. (4b) we can integrate symbolically and obtain:

$$\tilde{\varepsilon}_A(E) = 1 + \sum_j \frac{B_j}{E_j^2 - (E + ia)^2} = 1 + \sum_j \frac{B_j}{E_j'^2 - E^2 - 2iaE} \tag{7}$$

where $\tilde{\varepsilon}_A$ stands for the model free of divergences and $E_j'^2 = E_j^2 + a^2$. Hence, by using Eq. (4b) Sellmeier model has been turned into a sum of Lorentz oscillators, where the broadening parameter a equals the oscillator's half-width. The middle term of Eq. (7) can be understood as if the dielectric function had been shifted downwards in the complex plane by an amount of ia, so that the divergence has been removed from the real axis and relocated in the lower half plane, in what reminds Adachi's procedure. In Eq. (7), broadening is defined by a single parameter a that is common to all resonances E_j. Based on the additive terms in the expression of Eq. (6) and on the convolution property of linearity, we could assign a specific broadening parameter to each resonance by replacing a common parameter a with a specific one a_j per resonance.

Fig. 1 plots ε_1-1 for a Sellmeier model with one resonance at photon energy 1 eV, along with ε_1-1 and ε_2 for the Lorentz oscillator obtained from Sellmeier model with parameter a=0.01 eV. The unrealistic divergence of Sellmeier model at the resonant energy is removed with the Lorentz oscillator. Sellmeier model increasingly separates from the Lorentz oscillator when approaching the divergence.

Summarizing, as intuitively it could have been anticipated, a series of Lorentz oscillators is the divergenceless model that corresponds to Sellmeier model. In the simplest case, a single parameter a is enough to obtain a correct mathematical model; in a more practical case, a single parameter per resonance a_i is enough, with an increase in the number of parameters of only one per resonance (the broadening parameter) over Sellmeier original model involving divergences. The resulting sum of Lorentz oscillators not only lacks divergences, but additionally provides ε_2, which is not given by Sellmeier model; ε_2 for Sellmeier model would be a Dirac delta.

This single further parameter necessary to remove divergences from Sellmeier model contrasts with some empirical models that attempt to generalize Sellmeier or Cauchy models by including absorption; to do this, such models typically add three further fitting parameters, in addition to the three fitting parameters of n or ε_1 (in the case of Sellmeier model, three parameters per resonance) [23,24,25,26]. With these modified models, not only the imaginary optical constant is not consistent since it is not obtained through KK analysis and the dielectric function keeps the divergences, but the model requires six parameters compared to four parameters (for a one-term Sellmeier model) for the simpler and divergenceless Lorentz oscillator. The same result, i.e., a Lorentz oscillator, would be obtained if we started with a Lorentzian profile for the imaginary part of the dielectric function as the weight function in Eq. (4a) or Eq. (A.1a).

When the profile is closer to Gaussian, rather than Lorentzian, Brendel [19] developed a procedure to convolve the Gaussian profile with Lorentz oscillators. Brendel's procedure enables describing Voigt profiles, where a resonance is described by a convolution of a Gaussian and a Lorentzian function. Brendel's mechanism is equivalent to using a Gaussian weight function in the left term of Eq. (A.2a).

3.2. CL model

3.2.1 Model development

CL model [5] is a popular model that is not analytic and can be corrected with the present procedure, which is examined in this sub-section. Tauc-Lorentz (TL) is another popular non-analytic model [4], and it has already been turned analytic [16]. More generally, models described by a piecewise function are candidates to be corrected with the present procedure. Regarding Forouhi-Bloomer model [3], it has a further drawback: there is no decay of ε_2 at large energies, which cannot be solved by just applying the present method.

The present procedure is particularly suited to apply to CL model, developed by Ferlauto *et al.* [6]. The Cody model [5] was proposed to parameterize the dielectric function of amorphous semiconductors; it is based in that the shape of interband absorption onset is closely consistent with the assumption of parabolic bands and a constant dipole matrix element. Ferlauto *et al.* [6] improved that model to get the correct asymptotic behaviour at large energies. Such model is usually referred to as Cody-Lorentz model, CL. Ferlauto *et al.* also included the Urbach tail in the model.

Ferlauto's model describes ε_2 with the following expression:

$$\varepsilon_2 = \begin{cases} \dfrac{(E-E_g)^2}{(E-E_g)^2+E_p^2}\dfrac{AE_0\Gamma E}{\left(E^2-E_0^2\right)^2+\Gamma^2E^2}, & E \geq E_t \\ \dfrac{A_u}{E}\exp\left(\dfrac{E}{E_u}\right), & E < E_t \end{cases} \tag{8}$$

Eq. (8) involves six parameters (A, Γ, E_0, E_g, E_p, E_t) that must be obtained in the fit. E_t stands for the energy at which functionality changes between the Lorentz-type term and the Urbach term; A_u and E_u are defined for both ε_2 and its first derivative to be continuous at E_t, and they are obtained as a function of the fitting parameters. Ferlauto's model obtains ε_1 with KK analysis and it requires the addition of a seventh fitting parameter $\varepsilon_{1,\infty}$. The insertion of the Urbach tail in CL model with a piecewise function makes this model non-analytic. The model has also problems with parity due to the term E-E_g. It is noted that the second and higher derivatives of ε_2 are not continuous at E_t, which is a manifestation of the lack of analyticity. Furthermore, the term $\varepsilon_{1,\infty}$ makes inconsistent the expression for ε_1, since ε_1-1 and ε_2 should be directly related through the KK analysis with no subsequent fitting parameter. These shortcomings are solved with the present procedure.

One further shortcoming of Eq. (8) is the divergence at E=0. To avoid it, we redefine ε_2 in the energy range below E_t:

$$\varepsilon_2 = \begin{cases} \dfrac{(E-E_g)^2}{(E-E_g)^2+E_p^2}\dfrac{AE_0\Gamma E}{\left(E^2-E_0^2\right)^2+\Gamma^2E^2}, & E \geq E_t \\ A_u E\exp\left(\dfrac{E}{E_u}\right), & E < E_t \end{cases} \tag{9}$$

The change in the functionality of the Urbach tail does not involve any loss in the capacity to fit exponential tails and the new function avoids Ferlauto's model undesired feature of ε_2 to unphysically increase towards zero energy. ε_2, as defined in Eq. (9), was used as the weight function in Eq. (A.1a); the function with inverted sign was used for negative energies. The resulting integral could be solved symbolically and the result is presented here:

$$\widetilde{\varepsilon}_A(E) = \widetilde{\varepsilon}_{CL,A}(E) + \widetilde{\varepsilon}_{U,A}(E) \tag{10}$$

$\widetilde{\varepsilon}_A$ stands for the obtained analytic model. The first (second) additive term in the right hand side of Eq. (10) contains the analyticized function coming from CL (Urbach) functionality.

$$\tilde{\varepsilon}_{CL,A}(E)=1-\frac{AE_0\Gamma}{\pi}\left\{F(b,d_-,d_+;h_+,h_-,E_g,E_t)+F(d_-,d_+,b;h_+,h_-,E_g,E_t)+F(d_+,b,d_-;h_+,h_-,E_g,E_t)\right.$$
$$\left.+l(h_+,b,d_-,d_+,E_p)\left(\frac{\pi}{2}+i\log E_p\right)+l(h_-,b,d_-,d_+,E_p)\left(\frac{\pi}{2}-i\log E_p\right)\right\} \tag{11}$$

$$\tilde{\varepsilon}_{U,A}=\frac{A_u b}{\pi}\left[\exp\left(\frac{b}{E_u}\right)Ei\left(\frac{E_t-b}{E_u}\right)-\exp\left(\frac{-b}{E_u}\right)Ei\left(\frac{E_t+b}{E_u}\right)+\exp\left(\frac{-b}{E_u}\right)Ei\left(\frac{b}{E_u}\right)-\exp\left(\frac{b}{E_u}\right)Ei\left(\frac{-b}{E_u}\right)\right]+$$
$$\frac{2E_u A_u}{\pi}\left[exp\left(\frac{E_t}{E_u}\right)-1\right] \tag{12}$$

$$b(E)=E+ia \tag{13}$$

$$d_\pm=\sqrt{4E_0^2-2\Gamma^2\pm 2i\Gamma\sqrt{4E_0^2-\Gamma^2}} \tag{14}$$

$$h_\pm = E_g \pm iE_p \tag{15}$$

$$F(\alpha,\beta,\gamma;h_+,h_-,E_g,E_t)=\frac{\alpha(E_g-\alpha)^2\log(E_t-\alpha)}{(\alpha^2-\beta^2)(\alpha^2-\gamma^2)(\alpha-h_+)(\alpha-h_-)}-\frac{\alpha(E_g+\alpha)^2\log(E_t+\alpha)}{(\alpha^2-\beta^2)(\alpha^2-\gamma^2)(\alpha+h_+)(\alpha+h_-)} \tag{16}$$

$$l(h_\pm,b,d_-,d_+,E_p)=\frac{E_p h_\pm^2}{(h_\pm^2-b^2)(h_\pm^2-d_-^2)(h_\pm^2-d_+^2)} \tag{17}$$

$$A_u=\frac{A\Gamma E_0(E_t-E_g)^2\,exp\left(-\frac{E_t}{E_u}\right)}{\left[E_0^4+(E_t^2-2E_0^2+\Gamma^2)E_t^2\right]\left[E_p^2+(E_t-E_g)^2\right]} \tag{18}$$

$$E_u=\frac{p_4\left[E_0^4+E_t^4-(2E_0^2-\Gamma^2)E_t^2\right](E_t-E_g)}{4E_t^3(E_g-E_t)^3+p_1E_t^4+4p_2E_gE_t^3+2p_3E_gE_t(2E_0^2-\Gamma^2)+2E_p^2E_0^4} \tag{19}$$

$$\left.\begin{aligned} p_1&=-2E_p^2+4E_0^2-2\Gamma^2\\ p_2&=E_p^2-3E_0^2+\frac{3}{2}\Gamma^2\\ p_3&=3E_gE_t-E_g^2-E_p^2\\ p_4&=E_p^2+(E_t-E_g)^2 \end{aligned}\right\} \tag{20}$$

Note that the energy variable is present through *b* defined in Eq. (13). *Ei* stands for the exponential integral function [27,28]:

$$Ei(z)=-\int_{-z}^{\infty}\frac{e^{-t}}{t}dt,\quad |arg(z)|<\pi \tag{21}$$

Function Ei(z) is included in commonly-used mathematical software packages, such as Mathematica, MATLAB, and Maple.

The new function given by Eqs. (10) to (12) is analytic both on the real axis and in the upper complex half plane. The present analytic function bears some resemblance to the analytic function obtained for the Tauc-Lorentz model [16].

All parameters of the present analytic model are as per Ferlauto's model, except $\varepsilon_{1,\infty}$, which is not present any more, and a, which is added as a new parameter; hence the total number of parameters has not changed. Parameter $\varepsilon_{1,\infty}$ in Ferlauto's model was added to encompass contributions from outside the main spectral range covered by the model. Whilst such addition may not be necessary for many materials, the problem can be faced in a different way when that contribution is not negligible. Contributions may come from larger energies, such as inner electronic transitions, or smaller energies, such as reststrahlen or other infrared bands. Those features, being far away in energy, could be modelled with one or few Lorentz oscillators, which, added to the present model, would remain a self-consistent, fully analytic model.

The main contributions of the model presented in Eqs. (10) to (12) are:

- The function is analytic, hence mathematically correct, versus Ferlauto's model. This results in that the present function satisfies the conditions to describe the optical constants of a real material, so that experimental data can be expected to be more accurately fitted when we employ the analytic model.

- The second and higher derivatives are continuous, whereas in Ferlauto's model there is a discontinuity starting at the second derivative in the connection between the CL term and the Urbach tail.

- The function includes an Urbach tail, as Ferlauto's model, but the present function converges to zero at zero energy. Hence the present function can be extended all the way to zero energy. In fact, the divergence at E=0 had been removed before applying the present analyticizing procedure through the redefinition of ε_2 weight function given by Eq. (9), and the application of the present procedure keeps convergence at E=0.

An important advantage of the new function is that it is a single expression for the dielectric function, so that in principle all parameters of the model can be fitted with experimental data of either ε_1, ε_2, or both, whereas in Ferlauto's model, $\varepsilon_{1,\infty}$ is obtained only from ε_1 data and E_g is obtained basically from ε_2 data. Furthermore, $\tilde{N} = n + ik = \tilde{\varepsilon}^{1/2}$ can be also obtained right away from Eqs. (10) to (12) and hence in principle all parameters of the model can be also fitted with experimental data of either n or k. Anyway, ε_2 or k more strongly depend on E_g parameter than the corresponding real parts and hence E_g is more accurately obtained from data of ε_2 or k. The potential to fit the model with only k data is high, since it is probably the most commonly measured parameter of a material.

The present model enables calculating the optical constants of the material also for complex photon energies, more specifically, in the upper complex half plane. This benefit is useful in applications such as calculations connected with the Casimir effect, where the Casimir force is calculated in terms of the dielectric function at some specific imaginary energies [29]. The continuation of the optical constant function from the real axis to the upper complex half plane can be only performed if the optical function is analytic over the real axis. Such continuation is not possible for a piecewise function.

3.2.2 The new model applied to the optical constants of boron

In this subsection, the new function is applied to fit the experimental optical constants of boron. B films are an example of an amorphous semiconductor that can be fitted with the present model. A comprehensive characterization of B films deposited by evaporation was reported by Fernández-Perea *et al.* [30]. Data reported in Ref. [30] were used to fit the present model. Table 1 presents the fitting parameters, both with the present model and with Ferlauto's model.

Fig. 2 plots the experimental optical constants of B films and the fit both with Ferlauto's model and with the present analytic model. A large difference is observed for ε_2 at small energies, due to the different functionality used in the weight function to obtain the analytic model. Hence a realistic asymptotic behavior for ε_2 is obtained with no loss of fitting capacity elsewhere. Although not visible in the figure, Ferlauto's function for ε_1 also diverges at E=0, whereas the present function remains flat.

The most significant difference between the analytic and the non-analytic model is found close to the connection energy between the two functionalities involved in Ferlauto's model. Fig.3 plots the second derivative of the model for ε_1 and ε_2 in the spectral range around E_t. The discontinuity of ε_2 in Ferlautos's model at E_t is noticeable. The present analytic model and its derivative to any order are continuous; however, the oscillation observable in the new analytic model at E_t must be an artifact of the procedure used to develop the model starting with two functionalities. The second derivative of ε_1 does not have any discontinuity in Ferlauto's model; nonetheless, it has a very sharp unphysical feature, which is highly relaxed, although still present, with the current analytic model. The above discontinuity and the strong feature are smoothened through integration with parameter a; hence the larger the parameter a, the larger the smoothening of these

features. The referred features both in ε_1 and ε_2 appear somewhat shifted between the two models because the experimental data were independently fitted with each model.

Conclusions

A procedure has been developed to turn an optical-constant model that is non-analytic into analytic by using the model as a weight function in an integral over the spectrum with broadening functions $1/(E'-E-ia)$. Specific expressions have been obtained that enable one to use either the dispersion or the absorption part of the optical constants as the weight function to generate the full complex function. Integration results in the smoothening of the optical function through averaging it (by means of a convolution) with a Lorentzian function with a half-width that can be made as small as necessary (but not zero); hence this smoothening can be made mostly negligible. Choices of optical functions are the complex dielectric function, the complex refractive index and their inverse functions.

The procedure is applied on models that are non-analytic. One target group of models includes those that are described with a piecewise function, such as models for semiconductors involving a functionality change close to the energy gap, which includes TL or CL models. Another target group of models includes those with poles in the upper complex half plane or with divergences at infinite energies in this same half plane. Finally, a third target group are models that, although analytic, yet they have simple poles in the real axis, such as Sellmeier model; the present procedure enables removing these divergences too.

The procedure has been exemplified to turn CL model into analytic and to remove the divergences from Sellmeier model. The procedure turns Sellmeier model into a sum of Lorentz oscillators, with the benefit that absorption is also described with the addition of a single extra fitting parameter per resonance. CL model developed by Ferlauto *et al.* [6] was transformed into an analytic model with the same number of parameters. The analyticized CL model is differentiable to any order, whereas CL model has a discontinuity already in the second derivative. A modification in the Urbach tail part of CL model was performed to avoid the divergence at zero energy. The compact function of the new model enables fitting data not only of ε_2, but also of k. The analyticized CL model was applied to fit boron film optical constants.

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Appendix

The known parity of ε_1 and ε_2 can be explicitly introduced in Eqs. (4) and (5). The following equation makes use of this parity starting with Eq. (4):

$$\frac{2}{\pi}\int_0^\infty \frac{E'\varepsilon_2(E')}{E'^2-E^2+a^2-2iaE}dE' = \int_{-\infty}^{\infty}\left[\tilde{\varepsilon}(E')-1\right]\frac{a/\pi}{a^2+(E'-E)^2}dE' = \tilde{\varepsilon}_A(E)-1 \text{ (dielectrics)} \quad \text{(A.1a)}$$

$$-\frac{2i}{\pi}(E+ia)\int_0^\infty \frac{\varepsilon_1(E')-1}{E'^2-E^2+a^2-2iaE}dE' = \int_{-\infty}^{\infty}\left[\tilde{\varepsilon}(E')-1\right]\frac{a/\pi}{a^2+(E'-E)^2}dE' = \tilde{\varepsilon}_A(E)-1 \text{ (dielectrics)} \quad \text{(A.1b)}$$

The denominator in the left term of Eqs. (A.1) only differs from the one of a Lorentz oscillator in the a^2 term. Hence functions $1/(E'-E-ia)$ are very close to Lorentz oscillators when a is small. Additionally, a change of variables in Eqs. (A.1) enables expressing the left term as an integral of Lorentz oscillators without requesting a to be small:

$$\frac{2}{\pi}\int_0^\infty \frac{E'\varepsilon_2(E')}{E'^2-E^2-2iaE}dE' = \int_{-\infty}^{\infty}\left[\tilde{\varepsilon}(E')-1\right]\frac{a/\pi}{a^2+(E'-E)^2}dE' = \tilde{\varepsilon}_A(E)-1 \text{ (dielectrics)} \quad \text{(A.2a)}$$

$$-\frac{2i}{\pi}\left(\bar{E}+i\bar{a}\right)\int_0^\infty \frac{\varepsilon_1(E')-1}{E'^2-E^2-2iaE}dE' = \int_{-\infty}^{\infty}\left[\tilde{\varepsilon}(E')-1\right]\frac{a/\pi}{a^2+\left(E'-E\right)^2}dE' = \tilde{\varepsilon}_A(E)-1 \text{ (dielectrics)} \quad \text{(A.2b)}$$

where:

$$\bar{E}^2(E,a)=\frac{2a^2E}{\sqrt{E^2+4a^2}-E}, \quad \bar{a}^2(E,a)=\frac{E}{2}\left(\sqrt{E^2+4a^2}-E\right) \quad \text{(A.3)}$$

When a is small, $\bar{E}$ and $\bar{a}$ approach E and a, respectively, so that Eqs. (A.2) would reproduce Eqs. (A.1) since the term a^2 in the denominator could be neglected.

All the above developments can be reproduced by replacing $\tilde{\varepsilon}=\varepsilon_1+i\varepsilon_2$ with $\tilde{N}=\tilde{\varepsilon}^{1/2}=n+ik$ or even their inverse functions. Hence it is:

$$\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{k(E')}{E'-E-ia}dE' = \int_{-\infty}^{\infty}\left[\tilde{N}(E')-1\right]\frac{a/\pi}{a^2+\left(E'-E\right)^2}dE' = \tilde{N}_A(E)-1 \text{ (dielectrics)} \quad \text{(A.4a)}$$

$$-\frac{i}{\pi}\int_{-\infty}^{\infty}\frac{n(E')-1}{E'-E-ia}dE' = \int_{-\infty}^{\infty}\left[\tilde{N}(E')-1\right]\frac{a/\pi}{a^2+\left(E'-E\right)^2}dE' = \tilde{N}_A(E)-1 \text{ (dielectrics)} \quad \text{(A.4b)}$$

In the application of the present procedure to $\tilde{N}$ of metals, we can operate like with $\tilde{\varepsilon}$: we broaden just the part of the optical function that does not contain the pole, so that the broadened function keeps the same pole as the starting function. The derivation is straightforward; it is not given here for shortness.

Using the parity of the optical constants:

$$\frac{2}{\pi}\int_0^\infty \frac{E'k(E')}{E'^2-E^2+a^2-2iaE}dE' = \int_{-\infty}^{\infty}\left[\tilde{N}(E')-1\right]\frac{a/\pi}{a^2+\left(E'-E\right)^2}dE' = \tilde{N}_A(E)-1 \text{ (dielectrics)} \quad \text{(A.5a)}$$

$$-\frac{2i}{\pi}\left(E+ia\right)\int_0^\infty \frac{n(E')-1}{E'^2-E^2+a^2-2iaE}dE' = \int_{-\infty}^{\infty}\left[\tilde{N}(E')-1\right]\frac{a/\pi}{a^2+\left(E'-E\right)^2}dE' = \tilde{N}_A(E)-1 \text{ (dielectrics)} \quad \text{(A.5b)}$$

These expressions can be again modified to have Lorentz oscillator functions:

$$\frac{2}{\pi}\int_0^\infty \frac{E'k(E')}{E'^2-E^2-2iaE}dE' = \int_{-\infty}^{\infty}\left[\tilde{N}(E')-1\right]\frac{\bar{a}/\pi}{\bar{a}^2+\left(E'-\bar{E}\right)^2}dE' = \tilde{N}_A(E)-1 \text{ (dielectrics)} \quad \text{(A.6a)}$$

$$-\frac{2i}{\pi}\left(\bar{E}+i\bar{a}\right)\int_0^\infty \frac{n(E')-1}{E'^2-E^2-2iaE}dE' = \int_{-\infty}^{\infty}\left[\tilde{N}(E')-1\right]\frac{\bar{a}/\pi}{\bar{a}^2+\left(E'-\bar{E}\right)^2}dE' = \tilde{N}_A(E)-1 \text{ (dielectrics)} \quad \text{(A.6b)}$$

with $\bar{E}$ and $\bar{a}$ given by Eq. (A.3). All the presented formulae are summarized in Table A.1.

Figure Captions

Fig. 1. (color online) ε_1-1 for a Sellmeier model with one resonant photon energy at E_1=1 eV and B_1=1 eV^2, along with ε_1-1 and ε_2 for a Lorentz oscillator (LO) obtained from Sellmeier model with parameter a=0.01 eV.

Fig. 2. (color online) ε_1 (left) and ε_2 (right) of B films. Comparison of Ferlauto's model [6] and the present analytic model to fit experimental optical constants of Fernández-Perea *et al.* [30]

Fig. 3. (color online) The second derivative of ε_1 (left) and ε_2 (right) calculated with the fitting to the optical constants of B films both with Ferlauto's model and with the present analytic model in the spectral range around E_t.

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