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Procedure to convert optical-constant models into analytic

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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

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