

COMPENDIUM

Dispersion function of refractive index and extinction coefficient

INTRODUCTION

A dispersion model is required to correctly model the optical properties of a material as a function of photon energy or wavelength. The development of proper dispersion functions is a current topic of research, driven by the creation of novel materials. One may distinguish empirical models, like the Cauchy model, from those models that are grounded in elaborate solid state physics and are consistent with Kramers-Kronig relations KKR (or should be). Sometimes used are generalizations of those models, being KKR consistent but quite abstract. Although fitting the data well, the physical cause for using it might not always be clear. Also the empirical models find their justification, for example to characterize simple materials with few free parameters, or in process control, where a certain “quality” parameter may be monitored without the need for a physical meaning of that parameter. We refer the reader to various excellent textbooks on dispersion models, for example:

Harland G. Tompkins, Eugene A. Irene, (eds.) Handbook of Ellipsometry, William Andrew, Inc. 2005
 Claus F. Klingshirn, Semiconductor Optics, Springer Verlag, Berlin, Heidelberg 1995, 3rd Edition 2006

You can construct a dispersion function simply by adding various dispersion terms. Note that this superposition is only valid for the (complex) dielectric function ϵ but not for the complex index of refraction. This means that dispersion terms given as refractive index or absorption are internally converted to ϵ .

Most of the dispersion functions below are provided as the pure “terms”. It usually will be necessary to add “1”, or more generally ϵ_∞ to account for the high-energy response of the material. This may be done by adding an appropriate **eps_fix** term.

In the following, E denotes the photon energy.

90° do not transmit light (“crossed polarizers”, “no transmission” typically means a remaining background of 10^{-6})

Cauchy

The classical Cauchy dispersion formula for the refractive index is an empirical formula that may be used to describe essentially transparent media. It may be regarded as an approximation of the low-energy tail of oscillators (transitions) in the UV far away from the energy range of the instrument.

$$n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4}$$

In our implementation, an equivalent function is provided for the absorption $k(\lambda)$. Parameters are denoted by the suffix $_n$ or $_k$, respectively. The k -parameters default to zero.

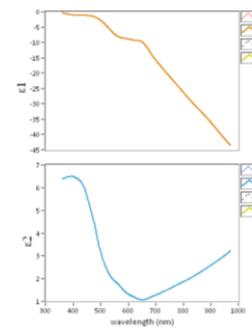


Figure 1. Dielectric function of gold

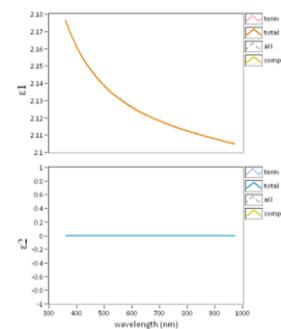


Figure 2. Dielectric function of SiO₂

Cauchy materials: Glass, transparent polymers, silicone oil,

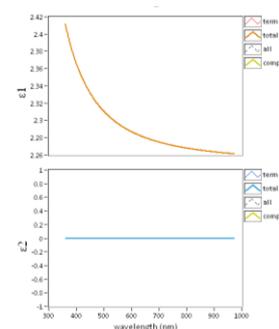


Figure 2. Cauchy function:

An = 1.4
 Bn = 3000
 Cn = 10⁸
 Ak = 0

Cauchy_Urbach

In an alternative, more physical implementation Cauchy_Urbach, $k(\lambda)$ may be represented by the Urbach formula

$$k(\lambda) = U_1 e^{U_2 \left(\frac{1239.84}{\lambda} - E_b \right)}$$

Note that E_b and U_1 are completely correlated, thus there are only 2 fittable parameters. Either E_b or U_1 are fixed and the other has to be adjusted or fitted accordingly.

Sellmeier, Sellmeier_term

This is an improvement of the classical Cauchy formula and valid for many transparent media.

$$n^2(\lambda) = 1 + \frac{B_1 \lambda^2}{\lambda^2 - C_1} + \frac{B_2 \lambda^2}{\lambda^2 - C_2} + \frac{B_3 \lambda^2}{\lambda^2 - C_3}$$

Sellmeier constants for many glasses and dielectrics are tabulated. Please note that the **Sellmeier** dispersion is the complete formula above for B and C parameters based on $[\lambda] = \mu\text{m}$. The **Sellmeier_term** is only a single term of the type

$$\varepsilon_i(\lambda) = \frac{B_i \lambda^2}{\lambda^2 - C_i}$$

under the same assumption for the magnitude of the parameters.

n_k_fix, eps_fix

Sets n & k or ε_1 & ε_2 as a wavelength-independent constant. This is sometimes useful if the dispersion of a material is expected to be low in a particular range. Eps_fix is also useful to set the high energy limit ε_∞ .

Pole_UV, Pole_IR

These terms represent a pole in the ε_1 function, according to

$$\varepsilon(E) = \frac{A}{E_0^2 - E^2}$$

These pole functions are identical except for their default center energies E_0 which are in the UV and IR, respectively. Please note that the poles must be outside of the instruments spectral range.

Lorentz

The classical Lorentz oscillator *term*, described by a resonance frequency E_0 , a strengths $f = AE_0$ and a damping Γ :

$$\varepsilon(E) = \frac{AE_0}{E_0^2 - E^2 - i \Gamma E}$$

Note that for a complete Lorentz oscillator model +1 has to be added (vis eps_fix) as an offset. Here we show only the pure term, allowing to add multiple oscillator terms without adding the offsets.

The Lorentz oscillator is a prototype to model many absorbing materials. A visually transparent material may be understood as Lorentz oscillators in the UV. One then sees the tail of the Lorentz dispersion function which looks like a Cauchy dispersion. To model the true situation, however, some refinements are necessary. For example, a band gap is not correctly represented by the Lorentz model. In a band gap material, ε_2 should become zero at energies below a band gap energy E_g and the material should become fully transparent then. This is not possible with the Lorentz oscillator.

Cauchy_Urbach materials: amorphous beryllium nitride, α -aluminum nitride, $\text{Ba}_{0.25}\text{Sr}_{0.75}\text{TiO}_3$ (transparent part of the spectra)

Sellmeier materials: Glass, sapphire, fused silica

Lorentz materials: layers with color center, plastic solar cells,

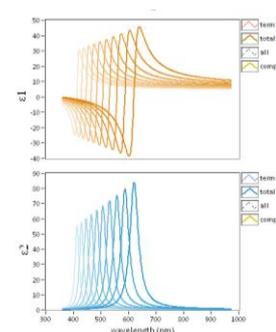


Figure 2. multiplot of Lorentz function:

$$E_0 = 2 - 3 \text{ eV}$$

$$f = 20 \text{ eV}^2$$

$$\Gamma = 0,1 \text{ eV}$$

Tauc_Lorentz, Tauc_Lorentz_Urbach, Cody_Lorentz

One refinement of the Lorentz oscillator is the Tauc-Lorentz oscillator (TL). It allows for a band gap, i.e. a non-absorbing region below the band gap energy E_g and describes the onset of absorption close to the band gap with a Tauc law:

$$\epsilon_2(E) = \begin{cases} 0; & E \leq E_g \\ G_T(E) \frac{AE_0\Gamma E}{(E_0^2 - E^2)^2 + \Gamma^2 E^2}; & E > E_g \end{cases}$$

where

$$G_T(E) = \frac{(E - E_g)^2}{E^2}$$

is the Tauc law.

Please note that the expression for $E > E_g$ is the product of the Tauc law and the imaginary part of the Lorentz oscillator.

The real part of the dielectric function, $\epsilon_1(E)$ is obtained from $\epsilon_2(E)$ by application of the Kramer-Kronig relations. The analytical expression is lengthy. The reader is referred to *Ferlauto et. al., J.Appl.Phys Vol 92, No. 5, 2002* for details.

Ferlauto et al. extend the TL Oscillator by implementation of an Urbach tail expression (TLU) for energies below the band gap:

$$\epsilon_2(E) = \begin{cases} \frac{E_1}{E} \exp\left\{\frac{(E - (E_t + E_g))}{E_u}\right\}; & E \leq (E_t + E_g) \\ \dots \text{as above}; & E > (E_t + E_g) \end{cases}$$

Herein, E_1 is a (internal) connection parameter required for continuity, given by

$$E_1 = (E_t + E_g)L(E_t + E_g)G_T(E_t + E_g)$$

Note that differing from Ferlauto et al. we introduce E_t as a (small) offset to E_g , rather than an absolute number. Thus, for comparison with the original definition one has

$$E_{t_Ferlauto} = E_t + E_g.$$

Another function derived by Cody to describe the behavior at the band gap onset

$$G_C(E) = \frac{(E - E_g)^2}{(E - E_g)^2 + E_p^2}$$

was proposed by Ferlauto et al., coming up with the Cody_Lorentz (CL) oscillator. E_p is an additional transition parameter to modify the transition region close to the band gap, separating the ‘‘Cody region’’ from the ‘‘Lorentz region’’. CL includes the Urbach tail already, so it is denoted as Cody_Lorentz_Urbach (CLU) in EP4Model.

For calculation speed, the Urbach tail contribution to $\epsilon_1(E)$ via KK has been omitted in TLU and CLU, leading to a small glitch in the $\epsilon_1(E)$ dispersion function at $E_t + E_g$.

TL, TLU and CLU are being used successfully for semiconductors, especially amorphous ones.

Materials: semiconductor

Drude

This oscillator is used for metals and models the resonance of the free electrons, i.e. a plasmon. It may be regarded as a special form of a Lorentz Oscillator. Its implementation is

$$\epsilon(E) = -\frac{A}{E^2 + i\Gamma E}$$

Tauc_Lorenz materials: amorphous materials in the interband region: amorphous oxide semiconductor,isolators and semiconductors

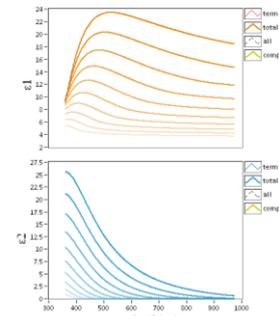


Figure 2. multiplot of Tauc_Lorentz function:

A = 125 eV
 $E_0 = 2,5 \text{ eV}^2$
 $\Gamma = 3,5 \text{ eV}$
 $E_G = 1 - 3 \text{ eV}$

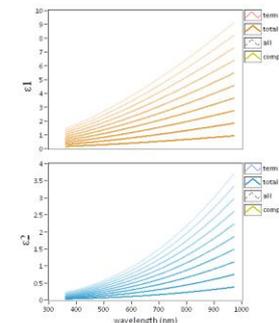


Figure 2. multiplot of Drude function:

A = $10^{20} - 10^{21} \text{ cm}^{-3}$
 $\Gamma = 0,5 \text{ eV}$

Drude materials: metals,

Here, A is related to the plasma energy $A = \epsilon_{\infty} E_p^2$, while Γ is a damping parameter.

Material: metals,

Forouhi_Bloomer

The Forouhi-Bloomer dispersion formula is being used also mainly for amorphous materials, starting from a function for $k(E)$

$$k(E) = \frac{A (E - E_g)^2}{E^2 - BE + C}$$

Besides the band gap energy E_g , there are 3 other fittable parameters. The real part of the refractive index, $n(E)$, is derived from this by a KK-type of integration, adding another free parameter n_{∞} (denoted as nhf) for the high frequency limit of the refractive index [Forouhi, Bloomer, 1986].

It has been argued by Jellison (2005) and others that the Forouhi-Bloomer formula is unphysical for several reasons. The reader is referred to the original literature for details.

Forouhi_Bloomer: amorphous materials, amorphous silicon, hydrogenated amorphous silicon, amorphous silicon nitride, and titanium dioxide [Forouhi, Bloomer, 1986]

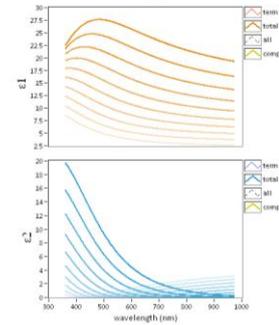


Figure 2. multiplot of Forouhi_Bloomer function:
 $A = 10^{20} - 10^{21} \text{ cm}^{-3}$
 $\Gamma = 0,5 \text{ eV}$