Cauchy and related Empirical Dispersion Formulae for Transparent Materials

Spectroscopic ellipsometry (SE) is a technique based on the measurement of the relative phase change of reflected and polarized light in order to characterize thin film optical functions and other properties. The measured data are used to describe a model where each layer refers to a given material. The model uses mathematical relations called dispersion formulae that help to evaluate the thickness and optical properties of the material by adjusting specific fit parameters.

This technical note deals with the Cauchy and related empirical transparent dispersion formulae to calculate the real (n) and imaginary (k) parts of the complex refractive index for a material.

Theoretical Model

Equation of Cauchy Transparent

The earliest dispersion formula was established by Cauchy (1836) who set up simple empirical dispersion law. The "Cauchy Transparent" dispersion works best when the material has no optical absorption in the visible spectral range and consequently generally has a normal dispersion which means a monotonous decreasing refractive index with increasing wavelength in this way:

$$1 < n(\lambda_{red}) < n(\lambda_{blue})$$

The following equation connects the refractive index to the wavelength (in nm):

$$\begin{cases} n(\lambda) = A + \dfrac{10^4 \cdot B}{\lambda^2} + \dfrac{10^9 \cdot C}{\lambda^4} \\ k(\lambda) = 0 \end{cases} \quad (1)$$

Equation of Cauchy Absorbent

A second formulation of the Cauchy model is the «Cauchy Absorbing» dispersion and it is more suitable to describe the optical properties of weakly absorbing materials. Here a non-zero extinction coefficient is given in an expression similar to the previous used for the refractive index:

$$\begin{cases} n(\lambda) = A + \dfrac{10^4 \cdot B}{\lambda^2} + \dfrac{10^9 \cdot C}{\lambda^4} \\ k(\lambda) = 10^{-5} \cdot D + \dfrac{10^4 \cdot E}{\lambda^2} + \dfrac{10^9 \cdot F}{\lambda^4} \end{cases} \quad (2)$$

The parameters of the equations

3 parameters are used in the equation of the Cauchy transparent model and 6 parameters in the Cauchy absorbing model.

Parameters describing the refractive index

- *A* is a dimensionless parameter: when $\lambda \to \infty$ then $n(\lambda) \to A$.
- *B* (nm^2) affects the curvature and the amplitude of the refractive index for medium wavelengths in the visible.
- *C* (nm^4) affects the curvature and amplitude for smaller wavelengths in the UV. Generally,

$$\boxed{0 < |C| < |B| < 1 < A \quad (3).}$$

3 parameters describe the extinction coefficient.

- *D* is a dimensionless parameter similar to *A*,
- *E* (nm^2) is analogous to *B*,
- *F* (nm^4) behaves like *C*.

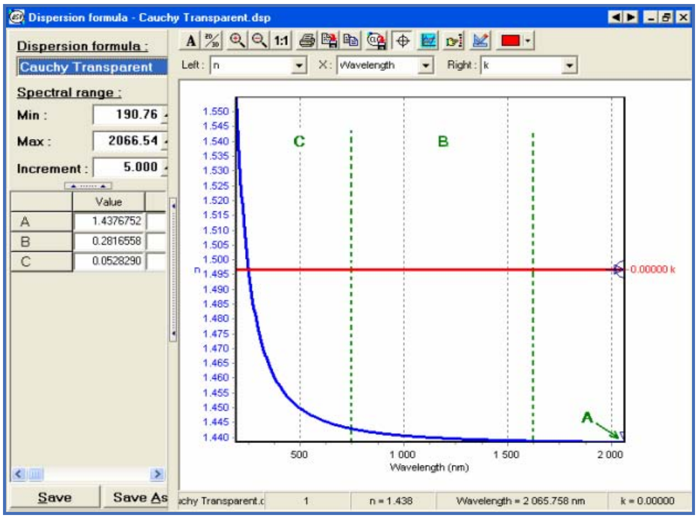
Limitation of the model

Cauchy's formulation cannot be easily applied to metals and semiconductors.

The parameters used do not have any physical meaning and therefore, these empirical relations are not Kramers-Kronig consistent. From first principles, the Kramers-Kronig relation relates the index of refraction and extinction coefficient parts; it means they are not independent quantities. In other words, if the value of the extinction coefficient is known over the entire spectral range, the index of refraction coefficient can be calculated.

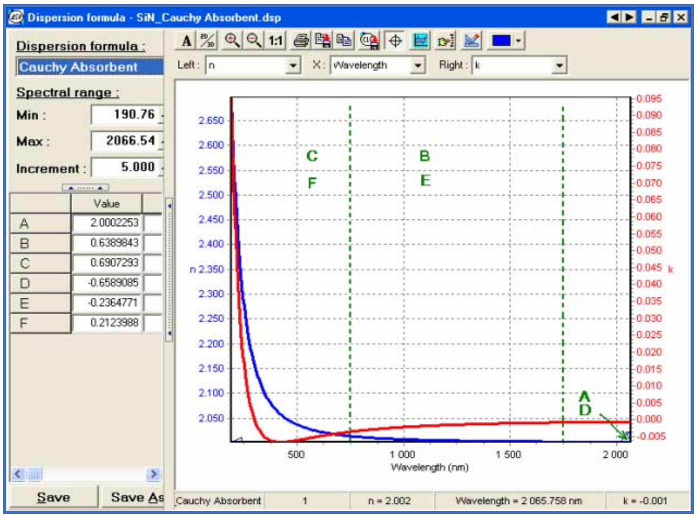
Parameter setup

Cauchy Transparent function



Optical properties of SiO_2 given by the Cauchy transparent function

Cauchy Absorbent function



Optical properties of SiN given by the Cauchy absorbent function

Application to materials

The Cauchy model is used for transparent materials like insulators, glasses exhibiting no or very low optical absorption in the Far Ultra Violet.

Materials	A	B	C	D	E	F	S.R (eV)
ChG Glass	6.5	0.7	0	0	0	0	
HfO	1.993	1.303	0.158	0	0	0	1.5 - 5.5
MgF	1.386	0.117	0.109	0	0	0	1.5 - 5.5
PI	1.631	0.497	1.337	771.776	- 0.587	1.117	
SiN	2.000	0.638	0.690	-0.658	-0.236	0.212	1 - 6.0
SiO_2	1.447	3660	0	0	0	0	1 - 6.0
TiO_2	2.374	1.932	6.855	0	0	0	1.5 - 6.0

References

1. L. Cauchy, Bull. des sc. Math., 14, 9 (1830).
2. http://en.wikipedia.org/wiki/Cauchy_equation.
3. G. Ghosh, Handbook of Thermo-Optic Coefficients of optical Materials with Applications, Academic Press.

Briot Dispersion Formula

Theoretical model

This dispersion model is based on a Laurent series (1864) expressing the equation for the refractive index of transparent materials:

$$n^2(\lambda) = A_0 + 10^{-2} \cdot A_1 \cdot \lambda^2 + \frac{10^{-2} \cdot A_2}{\lambda^2} + \frac{10^{-4} \cdot A_3}{\lambda^4} + \frac{10^{-6} \cdot A_4}{\lambda^6} + \frac{10^{-7} \cdot A_5}{\lambda^8} \quad (1)$$

with:

$$k(E) = 0 \quad (2).$$

The previous equation of the refractive index is also known as the *Schott* equation because it was used by the Schott company until 1992 when it was abandoned and replaced by the *Sellmeier* formula. However, Briot's equation remains widespread use elsewhere.

The parameters of the equations

Parameters describing the refractive index

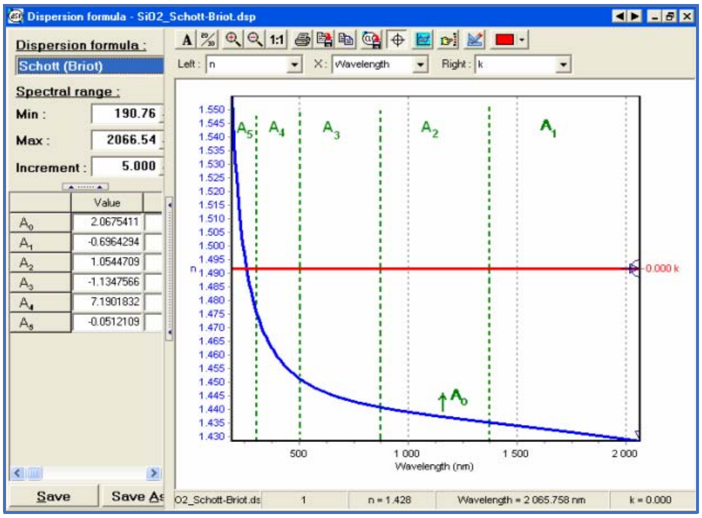
- A_0 (dimensionless), A_1 (in nm^{-2}), A_2 (in nm^2), A_3 (in nm^4), A_4 (in nm^6) and A_5 (in nm^8) are the different coefficients of the development in Laurent series.
- A_0 is a positive parameter that prevents $n^2(\lambda)$ from being negative.
- The low order terms of the development ($A_1 < 0$ and A_2) contribute to the intensity of the refractive index curve for long wavelengths in the visible and IR regions.
- The high order terms of the development (A_3, A_4 and A_5) contribute to the intensity of the refractive index curve for small wavelengths in the UV region.

Limitation of the model

Briot's formulation cannot be easily applied to metals and semiconductors.
This empirical relation is not Kramers-Kronig consistent and therefore does not have any physical meaning.

Parameter setup

Schott-Briot function



Optical properties of SiO_2 given by the Schott-Briot function

Application to materials

The Briot model is used for transparent materials such as crystalline quartz across the range 300nm~1600nm.

References

1. C. Briot, Essais sur la théorie mathématique de la lumière. Paris, Mallet-Bachelier, (1864).
2. www.optics.arizona.edu/Palmer/cgi-bin/index/dispeqns.pdf

Hartmann Dispersion Formula

Theoretical model

The Hartmann's (1926) model, has the following general form:

$$n(E) = A + \frac{C}{\lambda(E) - B} \quad (1)$$

This equation works for transparent films that do not have absorption:

$$k(E) = 0 \quad (2).$$

The parameters of the equations

3 parameters are used in the equation of the Hartmann model and allow to define the refractive index.

- *A* (*A* > 1) is a dimensionless parameter; when $\lambda \rightarrow \infty$ then $n(\lambda) \rightarrow A$.
- *B* and *C* have the dimension of wavelengths (nm).
- *B* is the resonance wavelength for which the refractive
- index diverges. The fit must be performed for wavelengths $\lambda \neq B$ otherwise $n(\lambda) \rightarrow \infty$.
- *C* determines the amplitude (strength) of the refractive index for wavelengths $\lambda \rightarrow B$.

Limitation of the model

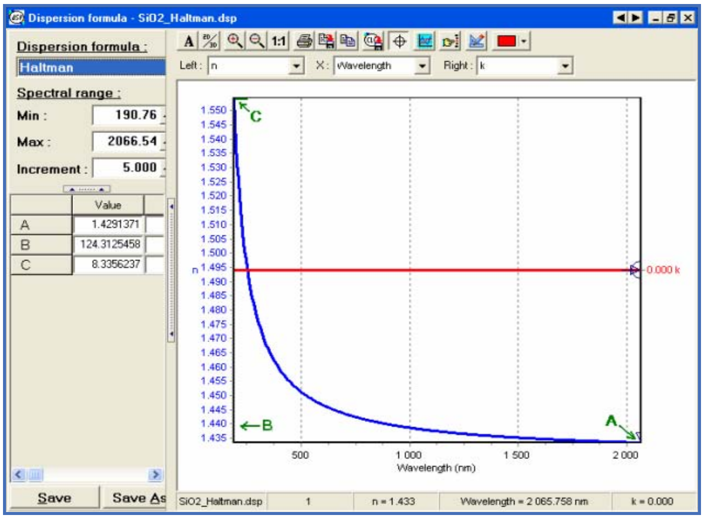
The Hartmann formula cannot be easily applied to metals and semiconductors.

This empirical formula is not Kramers-Kronig consistent and therefore does not have any physical meaning.

Parameter setup

The Hartmann function has similar application to the Cauchy Transparent dispersion. It is useful for transparent materials with normal dispersion.

Hartmann function



Optical properties of SiO_2 given by the Hartmann function

Application to materials

The Hartmann model is used for transparent materials like insulators, glasses.

Materials	A	B	C	S.R (eV)
SiO_2	1.429	124.312	8.335	0.7 - 6
TiO_2	1.890	178.621	203.804	1.5 - 4

References

1. http://scienceworld.wolfram.com/physics/HartmannDispersion-Formula.html
2. H. W. Lee, Trans. Opt. Soc., Volume 28, Issue 3, 161-167 (1926).
3. www.optics.arizona.edu/Palmer/cgi-bin/index/dispeqns.pdf

Conrady Dispersion Formula

Theoretical model

Conrady's equation (1960) allows the refractive index to be derived using the following equation for n(λ):

$$n(\lambda) = A + \frac{10^2 \cdot B}{\lambda} + \frac{10^9 \cdot C}{\lambda^{3.5}} \quad (1)$$

for a transparent film for which:

$$k(E) = 0 \quad (2).$$

The parameters of the equations

3 parameters are used in the expression of the *Conrady model*.

Parameters describing the refractive index

- *A* is a dimensionless parameter: when $\lambda \rightarrow \infty$ then $n(\lambda) \rightarrow A$.
- *B* (nm) has the same dimension as a wavelength. This parameter affects the curvature and amplitude of the refractive index for visible wavelengths.
- *C* ($nm^{3.5}$) influences the behaviour (strength) of the refractive index at small wavelengths in the UV.

Generally,

$$0 < |C| < |B| < 1 < A \quad (3)$$

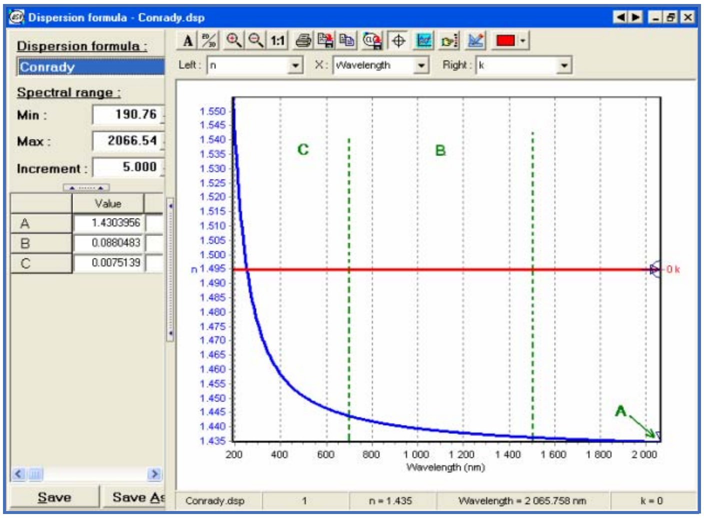
Limitation of the model

Conrady's equation cannot be easily applied to metals and semiconductors.
This empirical formula is not Kramers-Kronig consistent and therefore does not have any physical meaning.

Parameter setup

Conrady function has similar application to the *Cauchy Transparent formula*. It is useful for transparent materials with normal dispersion.

Conrady function



Optical properties of SiO_2 given by the Conrady function

Application to materials

The Conrady model is used for transparent materials like insulators, glasses.

Materials	A	B	C	S.R (eV)
SiO_2	1.427	0.111	0.00513	0.7 - 6
TiO_2	2,500	-1.148	0.731	1.5 - 4

References

1. A. E. Conrady, Applied Optics and Optical Design, Dover (1960).

Sellmeier Dispersion Formula

Theoretical model

Equation of Sellmeier Transparent

The Sellmeier formula (1871) is semi-empirical but it remains more accurate than the Cauchy dispersion law for characterizing the refractive index of a material across a wider spectral range. The transparent Sellmeier equation for the index of refraction looks like:

$$n^2(\lambda) = A + B \times \frac{\lambda^2}{\lambda^2 - \lambda_0^2} \quad (1)$$

without absorption:

$$k(\lambda) = 0 \quad (2)$$

Parameters of the Sellmeier Transparent function

3 parameters are used in the equation of the *Sellmeier Transparent model* to describe the refractive index variation.

Parameters describing the refractive index

- *A* ($1 \leq A$) is a dimensionless parameter that determines the value of the refractive index when when $\lambda \to \infty$ and B ~ 0. It represents the contribution of the ultraviolet term.
- *B* ($A \leq B$) is another dimensionless parameter that determines the shape of the refractive index in the visible range.
- λ_0 (in nm^2) is the resonance wavelength for which the refractive index diverges. The fit must be performed for wavelengths $\lambda \neq \lambda_0$ otherwise $n^2(\lambda) \to \infty$.

Equation of Sellmeier Absorbent

The Sellmeier Absorbent equation for the refractive index is written as follows:

$$n^2(\lambda) = \frac{1 + A}{1 + \frac{10^4 \cdot B}{\lambda^2}} \quad (3)$$

and the extinction coefficient is given by the relation below:

$$k(\lambda) = \frac{C}{10^{-2} \cdot n \cdot D \cdot \lambda + \frac{10^2 \cdot E}{\lambda} + \frac{1}{\lambda^3}} \quad (4)$$

Parameters of the Sellmeier Absorbent function

2 parameters describe the refractive index

- *A* is a dimensionless parameter that is linked to the amplitude of the refractive index. When $\lambda \to \infty$ then $n(\lambda) = \sqrt{1 + A}$.
- *B* (in nm^2) has an influence on the curvature of the refractive index: if $B > 0$, n increases with λ and the bigger *B* is the more straight $n^2(\lambda)$ is. If $B < 0$, n decreases with λ.

3 parameters describe the extinction coefficient

- *C* is a dimensionless parameter that determines the strength of the absorption coefficient curve.
- *D* (nm^{-1}) and *E* (nm) are terms corresponding to a development series similar to that of Schott-Briot formula. Increasing *D* and *E* involves a decrease of the absorption coefficient.

Limitation of the model

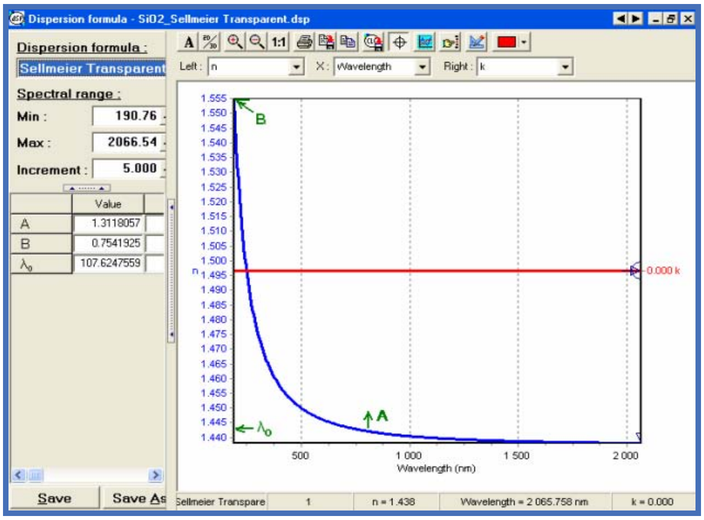
Sellmeier equations cannot be easily applied to metals and semiconductors.

These empirical relations are not Kramers-Kronig consistent and therefore do not have any physical meaning.

Parameter setup

The Sellmeier Transparent function behaves like the *Cauchy Transparent function*. It exhibits normal dispersion, so the refractive index decreases with increasing wavelengths.

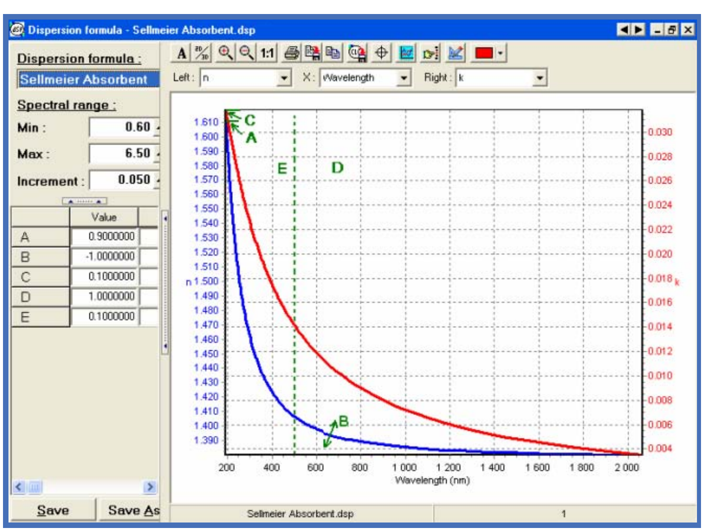
Sellmeier Transparent function



Optical properties of SiO_2 given by the Sellmeier Transparent function

The *Sellmeier Absorbent* function behaves like the *Cauchy Absorbing* function. This function also gives decreasing absorption and dispersion with increasing wavelength. Note that this is not physical in the presence of absorption as the Kramers-Kronig relation states that the refractive index should normally increase with increasing wavelength.

Sellmeier Absorbent function



Optical properties of a polymer given by the Sellmeier absorbent function

Application to materials

The Sellmeier model is used for transparent materials such as organics, insulators, glasses.

Valid spectral range

The Sellmeier equation mostly holds for wavelengths far from λ_0 in the range of transparency.

References

1. http://en.wikipedia.org/wiki/Sellmeier_equation
2. http://www.schott.com/optics_devices/english/download/tie-29_refractive_index_v2.pdf

Fixed Index Dispersion Formula

Theoretical model

The Fixed index dispersion formula is given by constant refractive index and extinction coefficient for any wavelength:

$$\boxed{\begin{cases} n(\lambda) = const. = n \\ k(\lambda) = const. = k \end{cases}}$$

The parameters of the equations

Only 2 parameters are needed to describe the model:

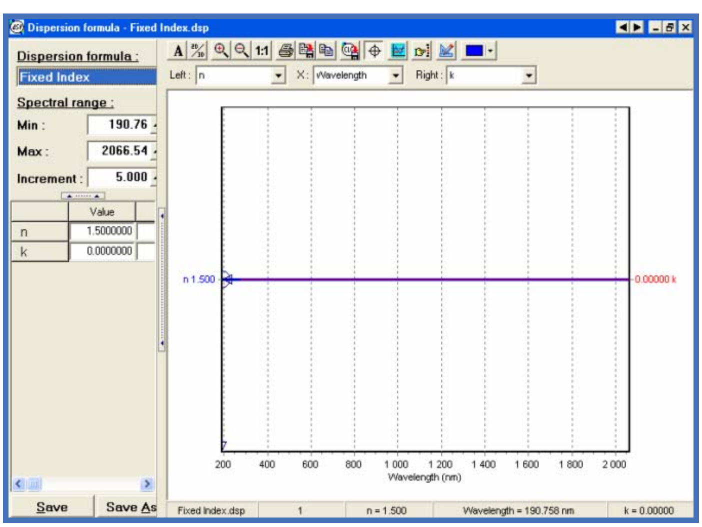
- *n* is the value of the refractive index.
- *k* is the value of the extinction coefficient.

Limitation of the model

This formula strictly describes the vacuum. The Fixed index equation does not apply to metals and semiconductors.

Parameter setup

Fixed index function



Fixed Index formula given a refractive index equal to 1.5

Application to materials

The *Fixed index* model is applicable to non dispersive materials like air. It is often used when the measurement is performed in different ambient media (liquids).

It can be used to decrease the number of fitting parameters when the material dispersion can be neglected.

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