Tauc-Lorentz Dispersion Formula

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 SE data are used to describe a model where layers refer to given materials. The model uses mathematical relations called dispersion formulae that help to evaluate the material's optical properties by adjusting specific fit parameters.

This technical note deals with Tauc-Lorentz dispersion formula.

Theoretical model

Jellison and Modine developed this model (1996) using the Tauc joint density of states and the Lorentz oscillator. The complex dielectric function is :

$$\widetilde{\varepsilon}_{TL} = \varepsilon_{r,TL} + i \cdot \varepsilon_{i,TL} = \varepsilon_{r,TL} + i \cdot \left(\varepsilon_{i,T} \times \varepsilon_{i,L} \right) \quad (1)$$

Here the imaginary part $\varepsilon_{i,TL}$ of the dielectric function is given by the product of imaginary part of Tauc's (1966) dielectric $\varepsilon_{i,T}$ function with Lorentz one $\varepsilon_{i,L}$. In the approximation of parabolic bands, Tauc's dielectric function describes inter-band transitions above the band edge as :

$$\varepsilon_{i,T}\left(E > E_g \right) = A_T \cdot \left(\frac{E - E_g}{E} \right)^2 \quad (2)$$

where :
- A_T is the Tauc coefficient
- E is the photon energy
- E_g is the optical band gap

The imaginary part of Tauc's dielectric function gives the response of the material caused by inter-band mechanisms only : thus $\varepsilon_{i,T} (E \leq E_g) = 0$.
The imaginary part of the Lorentzian oscillator model is given by :

$$\varepsilon_{i,L}(E) = \frac{A_L \cdot E_0 \cdot C \cdot E}{\left(E^2 - E_0^2 \right)^2 + C^2 \cdot E^2} \quad (3)$$

where :
- A_L is the strength of the $\varepsilon_{2,TL}(E)$ peak
- C is the broadening term of the peak
- E_0 is the peak central energy

By multiplying equation (2) by equation (3), Jellison sets up a new expression for $\varepsilon_{i,L}(E)$:

$$\varepsilon_{i,TL}(E) = \varepsilon_{i,L} \times \varepsilon_{i,T} = \begin{cases} \dfrac{1}{E} \dfrac{A E_0 C \left(E - E_g \right)^2}{\left(E^2 - E_0^2 \right)^2 + C^2 E^2} & \text{for } E > E_g \\[4mm] 0 & \text{for } E \leq E_g \end{cases} \quad (4)$$

where $A = A_T \times A_L$.

The real part $\varepsilon_{r,TL}$ of the dielectric function is derived from the expression of ε_i using the Kramers-Kronig integration. Then, it comes the following expression for ε_i:

$$\varepsilon_r(E) = \varepsilon_r(\infty) + \frac{2}{\pi} \cdot P \cdot \int_{E_g}^{\infty} \frac{\xi \cdot \varepsilon_i(\xi)}{\xi^2 - E^2} \, d\xi \quad (5)$$

where P is the Cauchy principal value containing the residues of the integral at poles located on lower half of the complex plane and along the real axis.
According to Jellison and Modine (Ref. 1), the derivation of the previous integral yields :

$$\begin{aligned} \varepsilon_{r,TL}(E) = \varepsilon_{\infty} &+ \frac{A \cdot C \cdot a_{\ln}}{2 \cdot \pi \cdot \zeta^4 \cdot \alpha \cdot E_0} \cdot \ln \left[\frac{E_0^2 + E_g^2 + \alpha \cdot E_g}{E_0^2 + E_g^2 - \alpha \cdot E_g} \right] \\ &- \frac{A}{\pi} \cdot \frac{a_{a\tan}}{\zeta^4 \cdot E_0} \cdot \left[\pi - \arctan\left(\frac{2 \cdot E_g + \alpha}{C} \right) + \dots \right. \\ &\qquad\qquad \left. + \arctan\left(\frac{\alpha - 2 \cdot E_g}{C} \right) \right] \\ &+ \frac{4 \cdot A \cdot E_0 \cdot E_g \cdot \left(E^2 - \gamma^2 \right)}{\pi \cdot \zeta^4 \cdot \alpha} \times \dots \\ &\times \left[\arctan\left(\frac{\alpha + 2 \cdot E_g}{C} \right) + \arctan\left(\frac{\alpha - 2 \cdot E_g}{C} \right) \right] \\ &- \frac{A \cdot E_0 \cdot C \cdot \left(E^2 + E_g^2 \right)}{\pi \cdot \zeta^4 \cdot E} \cdot \ln \left(\frac{|E - E_g|}{E + E_g} \right) + \dots \\ &+ \frac{2 \cdot A \cdot E_0 \cdot C}{\pi \cdot \zeta^4} \times E_g \cdot \ln \left[\frac{|E - E_g| \cdot \left(E + E_g \right)}{\sqrt{\left(E_0^2 - E_g^2 \right)^2 + E_g^2 \cdot C^2}} \right] \end{aligned} \quad (6)$$

where:

$$\begin{cases} a_{\ln} = \left(E_g^2 - E_0^2\right)\cdot E^2 + E_g^2 \cdot C^2 - E_0^2 \cdot \left(E_0^2 + 3\cdot E_g^2\right) \\ a_{a\tan} = \left(E^2 - E_0^2\right)\cdot\left(E_0^2 + E_g^2\right) + E_g^2 \cdot C^2 \\ \alpha = \sqrt{4\cdot E_0^2 - C^2} \\ \gamma = \sqrt{E_0^2 - C^2/2} \\ \zeta^4 = \left(E^2 - \gamma^2\right)^2 + \alpha^2 \cdot C^2/4 \end{cases} \quad (7)$$

Extension to multiple oscillators

In the case of multiple oscillators (N>1) the expression of ε_i contains now a series over all the oscillators.

$$\varepsilon_i = \begin{cases} \displaystyle\sum_{i=1}^{N} \frac{1}{E} \times \frac{A_i \cdot E_i \cdot C_i \cdot \left(E - E_g\right)^2}{\left(E^2 - E_i^2\right)^2 + C_i^2 \cdot E^2} & \text{for } E > E_g \\ 0 & \text{for } E \le E_g \end{cases} \quad (8)$$

and ε_r is re-written as the following sum :

$$\varepsilon_r(E) = \varepsilon_r(\infty) + \sum_{i=1}^{N} \frac{2}{\pi}\cdot P\cdot \int_{E_g}^{\infty} \frac{\xi\cdot\varepsilon_i(\xi)}{\xi^2 - E^2}\,d\xi \quad (9)$$

Deriving this integral yields the analytical expression of the real part of the dielectric function :

$$\begin{aligned}
\varepsilon_r(E) = \varepsilon_r(\infty) + \sum_{i=1}^{N} &\left\{ \frac{A_i \cdot C_i \cdot a_{\ln}}{2\cdot\pi\cdot\zeta^4\cdot\alpha\cdot E_i}\cdot\ln\left[\frac{E_i^2 + E_g^2 + \alpha\cdot E_g}{E_i^2 + E_g^2 - \alpha\cdot E_g}\right] \right. \\
&- \frac{A_i}{\pi}\cdot\frac{a_{a\tan}}{\zeta^4\cdot E_i}\cdot\left[\pi - \arctan\left(\frac{2\cdot E_g + \alpha}{C_i}\right) + \ldots \right. \\
&\qquad\qquad\qquad\left. + \arctan\left(\frac{\alpha - 2\cdot E_g}{C_i}\right)\right] \\
&+ \frac{4\cdot A_i \cdot E_i \cdot E_g \cdot\left(E^2 - \gamma^2\right)}{\pi\cdot\zeta^4\cdot\alpha}\cdot\left[\arctan\left(\frac{\alpha + 2\cdot E_g}{C_i}\right)\right. \\
&\qquad\qquad\qquad\left. + \arctan\left(\frac{\alpha - 2\cdot E_g}{C_i}\right)\right] \\
&- \frac{A_i \cdot E_i \cdot C_i \cdot\left(E^2 + E_g^2\right)}{\pi\cdot\zeta^4\cdot E}\cdot\ln\left(\frac{|E - E_g|}{E + E_g}\right) \\
&\left. + \frac{2\,A_i\,E_i\,C_i}{\pi\cdot\zeta^4}\,E_g\,\ln\left[\frac{|E - E_g|\left(E + E_g\right)}{\sqrt{\left(E_0^2 - E_g^2\right)^2 + E_g^2\,C_i^2}}\right]\right\} \quad (10)
\end{aligned}$$

The parameters of the equations

The name of the different Tauc-Lorentz formulae present in the DeltaPsi2 software depending on the number of oscillators are given below. It indicates the number of parameters too.

Formula	Number of oscillators	Number of parameters
Tauc-Lorentz	N=1	5
Tauc-Lorentz 2	N=2	8
Tauc-Lorentz 3	N=3	11

Increasing the number of oscillators leads to a shift of the peaks of absorption toward the ultraviolet region.

1 parameter is linked to the real part of the dielectric function

- $\varepsilon_r(\infty) = \varepsilon_\infty$ is the high frequency dielectric constant. This is an additional fitting parameter that prevents ε_1 from converging to zero for energies below the band gap. Generally, $\varepsilon_\infty > 1$.

At least 4 parameters describe the imaginary part of the dielectric function

- A_i (in eV) is related to the strength of the ith absorption peak. The subscript «i» refers to the number (i=1, 2 or 3) of oscillators. As A_i increases, the amplitude of the peak increases and the Full Width At Half Maximum (FWHM) of that peak gets slightly larger. Generally, $10 < A_i < 200$.
- C_i (in eV) is the broadening term ; it is a damping coefficient linked to FWHM of the ith peak of absorption. The higher it is the larger that peak becomes and at the same time the smaller its amplitude is. Generally $0 < C_i < 10$.
- E_g (in eV) is the optical band gap energy.
- E_i (in eV) is the energy of maximum transition probability or the energy position of the peak of absorption. The subscript «i» refers to the number (i=1, 2 or 3) of oscillators. Always, Eg<Ei.

Limitation of the model

The Tauc-Lorentz model requires ε_i to be zero for energies less than the band gap. Consequently, Tauc-Lorentz model does not take into account intra-band absorption: any defect or intra-band absorption increases ε_i below the band gap and generates bad fits in that region.

Valid spectral range

The Tauc-Lorentz model well describes the behaviour of materials for energies $E \le E_i$ where E_i is the transition energy of the oscillator of highest order.

Parameter setup

The Tauc-Lorentz model works particularly well for amorphous materials exhibiting an absorption in the visible and/or FUV range (absorbing dielectrics, semiconductors, polymers).

Note that :

- The graph below shows the different contributions (in red dashed lines) to the imaginary part of the Tauc Lorentz dielectric function (in red bold line).
- The sign «∝» before a given parameter means that either the amplitude or the broadening of the peak is linked to that parameter.

Tauc-Lorentz function
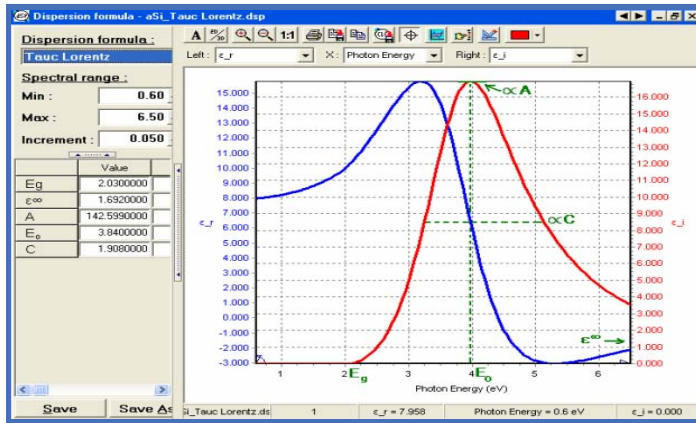
Dielectric function of a-Si represented by a single Tauc-Lorentz oscillator

Double Tauc-Lorentz function
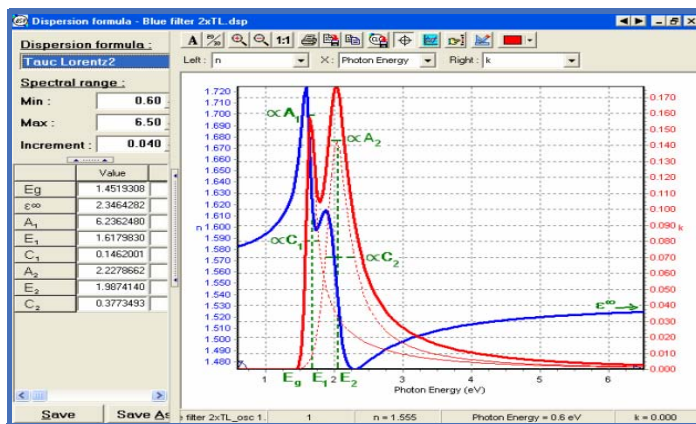
Dielectric function of a blue filter represented by a double Tauc-Lorentz oscillator

Applications to materials

Materials following the Tauc-Lorentz model

The asterisk * refers to parameters that are negative and thus do not have any physical meaning but represent good starting values to perform the fit on the material.

Materials	Eg	ε_∞	A	E_0	C	S. R. (eV)
a-C	1.305	3.774	38.835	6.335	6.227	1.5 - 5
AlGaN	3.300	3.000	100.000	4.500	1.000	1.5 - 2.5
As_2S_3	2.349	1.240	133.819	4.574	5.935	0.75 - 4.75
AsSSe	1.000	1.600	50.000	3.500	2.000	0.75 - 4.5
DLC	0.374	2.960	11.558	3.533	3.346	0.7 - 2
GaN	3.200	3.500	100.000	4.500	1.000	1,5 - 3
GeSbSe	1.851	2.062	54.703	3.412	2.045	0.65 - 3
InGaN	3.000	3.500	100.000	4.500	1.000	1,5 - 3
Polymer	3.027	1.701	32.921	5.759	2.416	0.7 - 4
poly-Si	0.882	3.937	49.597	3.711	0.321	1.5 - 3.25
a-Si	2.030	1.692	142.599	3.840	1.908	0.75 - 3.65
a-Si:B	1.267	2.148	143.380	3.617	1.994	0.75 - 4.75
a-Si:H	1.393	0.626	171.105	3.582	2.201	0.75 - 4.75
$Si_xO_yN_z$	3.864	1.760	77.340	8.363	3.550	1.5 - 6.5
Ta-C	1.395	2.558	67.312	8.713	9.760	1.5 - 5
ZnS	2.976	4.500	57.167	3.954	1.200	1.5 - 6.5
GeSbTe	0,450	2,024	158,795	1,688	2,397	0,65 - 3

Materials following the Double Tauc-Lorentz model

Materials	Eg	ε_∞	A_1	E_1
Blue Filter	1.451	2.346	6.236	1.617
Oxide coating	1.168	0.894	41.060	6.464
Polymer	3.420	2.771	113.260	4.234
SiC	1.521	-1.657*	4.026	5.678
Ta_2O_5	4.261	1.827	188.580	4.188

Materials	C_1	A_2	E_2	C_2	S. R. (eV)
Blue Filter	0.146	2.227	1.987	0.377	0.6 - 2.2
Oxide coating	4.140	-6.269*	3.763	2.390	1.5 - 5
Polymer	1.455	6.870	4.806	8.345	0.7 - 5
SiC	-5.129*	51.264	9.561	3.869	1.5 - 6.5
Ta_2O_5	5.278	58.367	5.354	1.246	1.5 - 6.5

Materials following the Triple Tauc-Lorentz model

Materials	Eg	ε_∞	A_1	E_1	C_1	A_2
a - Si	1.405	1.029	-16.227*	6.800	5.454	1.310
HfO_2	4.972	2.764	80.221	7.451	0.876	4.604

Materials	E_2	C_2	A_3	E_3	C_3	S. R. (eV)
a - Si	0.807	2.215	185.343	3.707	2.379	0.6 - 6
HfO_2	4.192	6.834	4.469	6.368	0.599	1.5 - 6.5

References

1) G.E. Jellison and F.A. Modine, Appl. Phys. Lett. 69 (3), 371-374 (1996).
2) Erratum, G. E. Jellison & F. A. Modine, Appl. Phys. Lett. 69 (14), 2137 (1996).
3) H. Chen, W. Z. Shen, Eur. Phys. J. B. 43, 503-507 (2005).

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