Classical Dispersion Model

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 application note deals with the classical dispersion formula. Note that more detailed explanation are given in the technical notes: Drude's and Lorentz dispersion model.

Theoretical model

The classical dispersion model is based on the sum of the single and double Lorentz, and Drude oscillators.

$$\tilde{\varepsilon}(\omega) = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\cdot\omega_t^2}{\omega_t^2 - \omega^2 + i\cdot\Gamma_0\cdot\omega} + \frac{\omega_p^2}{-\omega^2 + i\cdot\Gamma_d\cdot\omega} + \sum_{j=1}^{2}\frac{f_j\cdot\omega_{0j}^2}{\omega_{oj}^2 - \omega^2 + i\cdot\gamma_j\cdot\omega}$$

• Lorentz dispersion model

The Lorentz classical theory (1878) is based on the classical theory of interaction between light and matter and is used to describe frequency dependent polarization due to bound charge.

The Lorentzian dispersion formula comes from the solution of the equation of an electron bound to a nucleus driven by an oscillating electric field E. The response is equivalent to the classical mass on a spring which has damping and an external driving force. It generates damped harmonic oscillations.

In the DeltaPsi2 software the classical dispersion formula contains three oscillators.

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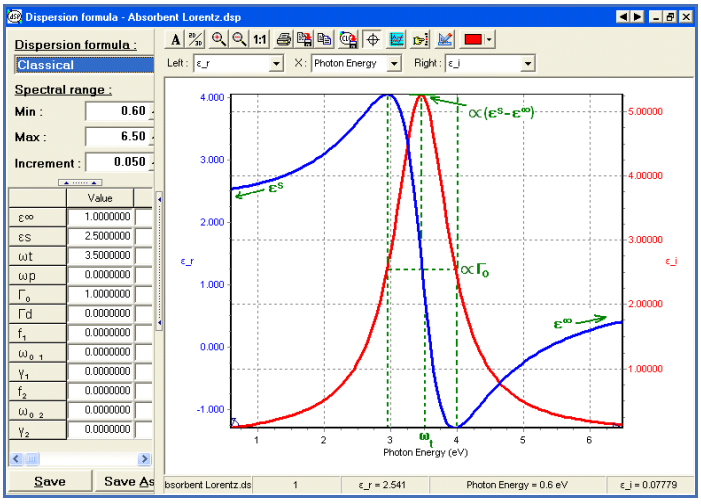


Single Lorentz oscillator

Parameters describing the real part of the dielectric function

- The constant ε_∞ is the high frequency dielectric constant. Generally, $\varepsilon_\infty = 1$ but can be greater than 1 if oscillators in higher enegies exist and are not taken into account.
- The constant ε_s ($\varepsilon_s > \varepsilon_\infty$) gives the value of the static dielectric function at a zero frequency. The difference $\varepsilon_s - \varepsilon_\infty$ represents the strength of the single Lorentz oscillator. The larger it is then the smaller the width Γ_0 of the peak of the single Lorentz oscillator.

Parameters describing the imaginary part of the single Lorentz oscillator dielectric function

- ω_t (in eV) is the resonant frequency of the oscillator whose energy corresponds to the absorption peak. When ω_t increases then the peak is shifted to higher photon energies. Generally, $1 \le \omega_t \le 20$.
- Γ_0 (in eV) is the broadening of each oscillator also known as the damping factor. The damping effect is due to the absorption process involving transitions between two states. On a graphic representing $\varepsilon_i(\omega)$, Γ_0 is generally equal to the Full Width At Half Maximum (FWHM) of the peak. As Γ_0 increases the width of the peak increases, but the amplitude of that decreases. Generally, $0 \le \Gamma_0 \le 10$.

Parameters describing the imaginary part of the multiple Lorentz oscillators dielectric function

- f_i (j = 1, 2 … N) term is the oscillator strength present in the expression of the multiple Lorentz oscillator. As fj increases then the peak amplitude increases, but the width of the peak γ_j decreases. Generally, $0 \le f_i \le 10$.
- ω_{0j} (in eV) (j = 1, 2 … N) is the resonant (peak) energy of an oscillator for a collection of several Lorentzian oscillators. It is similar to ω_t . Generally, $1 \le \omega_{0j} \le 8$.
- γ_j (in eV) (j = 1, 2 … N) parameter is the broadening parameter corresponding to the peak energy of each oscillator. It behaves like Γ_0 . Generally, $0 \le \gamma_j \le 10$.

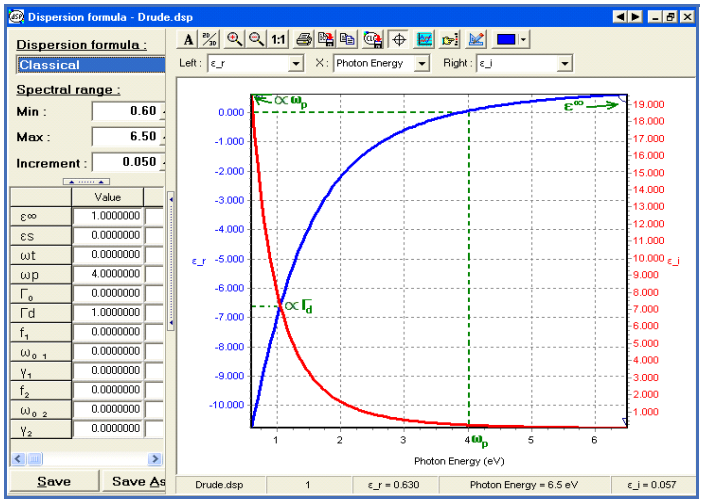
- Drude dispersion model

Drude's model (1900) is based on the kinetic theory of electrons in a metal which assumes that the material has motionless positive ions and a non-interacting electron gas. This simple model uses classical mechanical theory of free electron. It was constructed in order to explain the transport properties of conduction electrons in metals (due to intra-band transitions in a quantum-mechanical interpretation), conductive oxides and heavily doped semiconductors.

Since the conduction electrons are considered to be free, Drude oscillator is an extension of the single Lorentz oscillator to a case where the restoring force and the resonance frequency are null (Γ_0=0, ω_t = 0).

In the DeltaPsi2 software the classical dispersion formula contains the Drude model expressed as below:

$$\tilde{\varepsilon}(\omega) = \varepsilon_\infty + \frac{\omega_p^2}{-\omega^2 + i \cdot \Gamma_d \cdot \omega}$$



Classical Drude function

- ω_p is the plasma frequency corresponding to the photon energy position where $\varepsilon_r(\omega)$ is approximately zero. When ω_p increases then the amplitude of the $\varepsilon_r(\omega)$ and $\varepsilon_i(\omega)$ increases too.

$$\omega_p = \sqrt{\frac{N \cdot e^2}{m \cdot \varepsilon_0}}$$

- Γ_d (in eV) is the collision frequency. As Γ_d increases the broadening of the absorption tail increases too. Generally, for metals $0.4 < \Gamma_d < 4$.

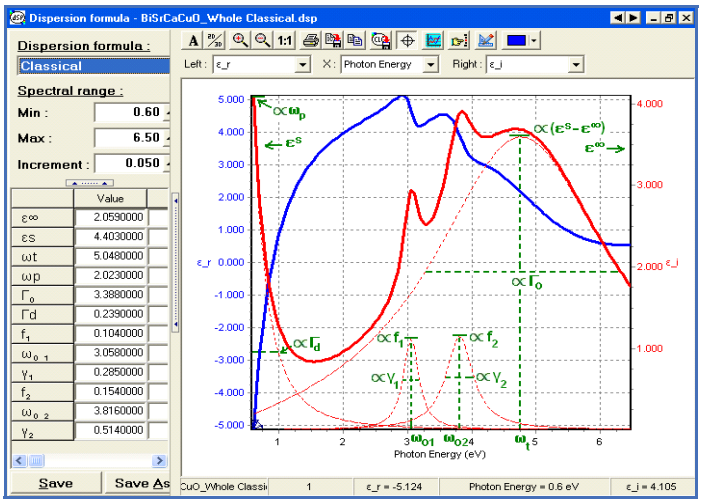
Application to Materials

The Lorentz oscillator model works well for insulators and semiconductors above the band gap.

The Drude model describes well the optical properties of metals but does not take into account the notion of optical band gap energy E_g .

The combination of both is often adequate when the material is a little conductive and has a metallic character (like conducting oxides ITO, RuO_2).

The graph above typically shows the influence of Drude's function characterized by an increasing absorption (imaginary part of the dielectric function) toward the IR region.



Dielectric function of BiSrCaCuO

List of materials following Drude and Lorentzian dispersion models

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	ε_∞	ε_s	ω_t	ω_p	Γ_0	Γ_d
Ag	-2.875*	3.401	9.6310	8.707	1.783	0.073
Al	0.959	16.787	1.637	13.320	0.705	0.119
Cr	3.9	4	0	20.000	0	100.000
Cu	1	1.65	1.80	4.00	3.00	0.85
IrO_2	1.0	6.209	6.650	3.989	9.002	0.819
ITO/PET	1.0	4.077	6.841	1.244	2.365	0.107
ITO/glass	3.201	4.039	4.935	1.850	0.302	0.0854
MoSi	1	7.948	6.628	2.714	9.081	7.870
NiCr	1	0.890	0	14.270	0	4.020
NiFe	1	0.880	0	14.790	0	4.780
Si_3N_4	1.0	5.377	3.186	0	0	0
SnO_2	0.714	0.792	4.933	7.814	1.141	15.546
Ta	1	1.790	0	21.530	0	19.799
TiN	1.348	3.610	5.067	4.769	6.339	4.343
YAG:Tb(10%)	1.0	2.545	10.342	0.793	0	0
$Y_3Fe_5O_{12}$	3.410	4.636	3.369	0.305	0.346	0.165
ZnO	1	2.900	7.250	5.450	2.700	17.150

List of materials following Drude and double Lorentz oscillator models

Materials	ε_∞	ε_s	ω_t	ω_p	Γ_0	Γ_d
Al	0.884	0	0	13.346	0	0.119
Au	-4.230*	6.956	8.481	7.971	7.449	0.078
BiSrCuO	2.059	4.403	5.048	2.023	3.388	0.239
C60	2.306	3.362	4.556	0.000	1.046	0.000
Cr	1.769	56.676	1.311	4.179	5.715	0.609
Cu	3.070	8.173	2.234	8.896	0.880	-0.047*
CuPC	2.551	0	0	0	0	0
Mo - Pal	2.216	10.869	4.190	8.306	2.048	0.347
p-Si	7.000	0	0	0	0	0
SiC - pal	2.922	6.401	6.843	0.000	0.974	0.000
Ta	1.129	2.617	3.140	7.683	1.527	0.045
Ti	-0.551*	0	0	5.415	0	1.942
TiN	3.050	0	0	12.071	0	11.321

Materials	f_1	$\omega_{0,1}$	γ_1	f_2	$\omega_{0,2}$	γ_2
Al	9.255	1.990	1.667	7.766	1.572	0.391
Au	-1.476*	0.182	4.243	-3.011*	6.619	2.692
BiSrCuO	0.104	3.058	0.285	0.154	3.816	0.514
C60	0.223	2.704	0.439	0.364	3.523	0.420
Cu	-6.330*	-2.137*	0.909	9.926	4.597	10.564
Cr	1.648	6.769	3.606	0	0	0
CuPC	0.425	2.022	0.210	0.149	3.574	0.334
Mo - Pal	3.093	1.712	0.557	11.119	2.426	1.475
p-Si	6.000	3.400	1.000	5.500	4.400	1.250
SiC - pal	0.154	2.403	2.188	0.080	4.042	1.203
Ta	-1.935*	-1.971*	0.926	18.717	7.896	26.969
Ti	0.300	-5.789*	-0.404*	2.102	-3.328*	2.203
TiN	-1.089*	2.006	1.026	0.929	4.743	1.011

References

1) H.M. Rosenberg, The Solid State, Oxford University Press.
2) F. Wooten, Optical Properties of Solids, Academic Press (1972).
3) Eugene Hecht, Optics, Addison-Wesley, NY (1997)
4) http://www.ifm.liu.se/~boser/surfacemodes/L3.pdf
5) langley.atmos.colostate.edu/at622/notes/at622_ sp06_sec13.pdf
6) F. Wooten, Optical Properties of Solids, Academic Press (1972)
7) H. M. Rosenberg, The Solid State, Oxford University Press (1988)
8) J. M. Cazaux, Introduction a la physique du Solide, Masson (199)
9) E. Hecht, Optics, Chap. 3, Hardcover (2001)
10) www.ece.tamu.edu/People/bios/hemmer_files/15-dispersion.ppt