Drude Dispersion Model

Spectroscopic Ellipsometry (SE) is a technique based on the measurement of the relative phase change of reflected polarized light in order to characterize thin film optical functions and other properties. The measured SE data is described by a model where layers refer to a given material. The model uses mathematical relations called dispersion formulas that help to evaluate the material's optical properties by adjusting specific fit parameters.
This technical note deals with the Drude dispersion formula.

Note that the technical notes «Classical dispersion model» and «Lorentz dispersion model» are complementary to this one.

Theoretical 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 ($\Gamma_0=0$, $\omega_t = 0$) - see «Lorentz dispersion model» technical note.

The equation of motion is:

$$m\cdot\frac{d\vec{v}}{dt}+m\cdot\Gamma_d\cdot\vec{v}=-e\cdot\vec{E} \quad (1)$$

where:

- m (d**v**/dt) is the acceleration force; m is the mass of the oscillator (here the electron) and v is the speed of the gas of electron;
- m Γ_d **v** is the friction force;
- the term -e.**E** is the electric force; it contains the term $E=E_0\, e^{i\omega t}$ which is the electric field of pulsation ω and -e which is the electric charge.

The solution of the previous equation is given by the following expression for oscillation amplitude:

$$\vec{v}(\omega)=\vec{v}_0\cdot e^{i\omega t}=\frac{-e}{m}\cdot\frac{\vec{E}_0}{i\omega+\Gamma_d} \quad (2)$$

The conduction density of current J_c corresponding to the movement of the N electrons per unit volume is:

$$\vec{J}_c(\omega)=-N\,e\,\vec{v}=\frac{N\,e^2}{m\cdot(\Gamma_d+i\,\omega)}\vec{E} \quad (3)$$

The displacement density of current of vacuum is expressed by:

$$\vec{J}_d=\frac{\partial\vec{D}}{\partial t}=i\,\omega\,\varepsilon_0\,\vec{E} \quad (4)$$

where **D** is the electric displacement of vacuum: $\mathbf{D} = \varepsilon_0\mathbf{E}$.

The total density of current **J** is given by:

$$\vec{J}(\omega)=\vec{J}_c+\vec{J}_d=\left[\frac{N\cdot e^2}{m\cdot(\Gamma_d+i\,\omega)}+i\,\omega\,\varepsilon_0\right]\vec{E} \quad (5)$$

Assuming that the plasma can also be characterized by identifying the total density of current to a global displacement current **Dtot** $= \varepsilon_0\varepsilon_r\mathbf{E}$. A new expression for the total density of current is then given by:

$$\vec{J}(\omega)=\frac{\partial\vec{D}_{tot}}{\partial t}=i\,\omega\,\varepsilon_0\,\tilde{\varepsilon}\,\vec{E} \quad (6)$$

The identification of the two last formulations of the total density of current **J** yields:

$$\vec{J}(\omega)=\left[\frac{N\cdot e^2}{m\cdot(\Gamma_d+i\,\omega)}+i\,\omega\,\varepsilon_0\right]\cdot\vec{E}=i\,\omega\,\varepsilon_0\,\tilde{\varepsilon}(\omega)\cdot\vec{E} \quad (7)$$

By simplifying that last expression, it is possible to deduce Drude's dielectric function ε(ω) given by the following equation:

$$\tilde{\varepsilon}(\omega)=1-\frac{N\,e^2}{m\,\varepsilon_0}\cdot\frac{1}{(\omega^2-i\Gamma_d\,\omega)}=1-\frac{\omega_p^2}{-\omega^2+i\cdot\Gamma_d\cdot\omega} \quad (8)$$

Note that for $\omega\to\infty$, $\varepsilon(\infty)\to 1$ then it is possible to re-write the dielectric function as:

$$\tilde{\varepsilon}(\omega)=\varepsilon(\infty)-\frac{\omega_p^2}{-\omega^2+i\cdot\Gamma_d\cdot\omega} \quad (9)$$

like in DP2 software, where ε(∞) is the high-frequency contribution that is usually superior or equal to one.

The real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$ parts of the dielectric function are given by:

$$\varepsilon_1(\omega) = 1(\varepsilon(\infty)) - \frac{\omega_p^2}{\omega^2 + \Gamma^2} \quad (10.1)$$

and

$$\varepsilon_2(\omega) = \frac{\omega_p^2 \cdot \Gamma}{\omega \cdot (\omega^2 + \Gamma^2)} \quad (10.2)$$

Behaviour of Drude dielectric function

- If $\omega < \omega_p$ then the real part of ε is negative: any electrical field cannot penetrate the metal that is totally reflective. **The optical constants of the material are complex.**
- If $\omega = \omega_p$ then the real part of the dielectric function is zero. This means that all electrons oscillate in phase throughout the material propagation length.
- If $\omega > \omega_p$ the reflectivity decreases and the metal becomes transparent. **The refractive index of the material is almost real.**
- When $\omega^2 >> \Gamma_d^2$ then $\varepsilon_r(\omega) = 1 - (\omega_p^2/\omega^2)$. The imaginary part of the dielectric function can be approximated by $\varepsilon_i(\omega) = (\omega_p^2\, \Gamma/\omega^2)$ and there is no absorption at the high frequency limit.

The parameters of the dispersion formula

2 parameters are used in the Drude's model. Both ω_p and Γ_d influence the real and imaginary parts of the dielectric function.

- ω_p is the plasma frequency. It corresponds to the photon energy position where $\varepsilon_r(\omega)$ is approximately zero. As ω_p increases the amplitude of $\varepsilon_r(\omega)$ 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. Generally, for metals $0 < \Gamma_d < 4$. As Γ_d increases the broadening of the absorption tail increases too.

Limitation of the model

The Drude oscillator describes well the optical properties of metals but does not take into account the notion of optical energy band gap E_g semiconductors and the quantum effects.

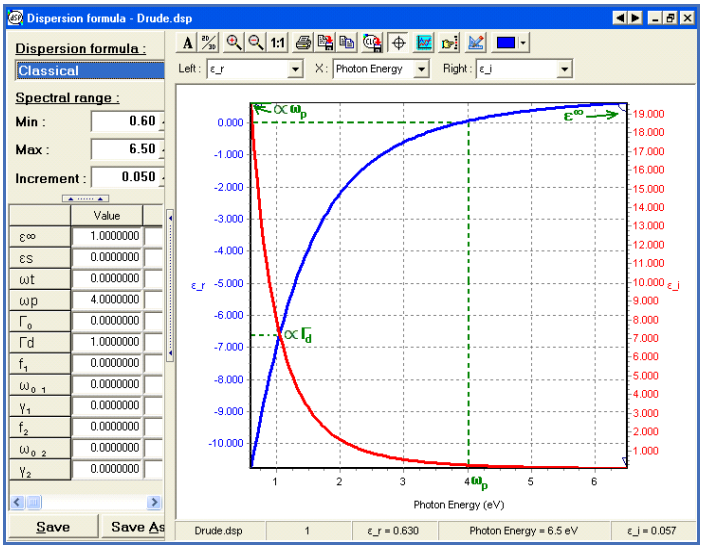
Parameter setup

Note that:

1 - The Drude's dielectric function is available in the Classical dispersion formula in the DeltaPsi2 software.

2 - The sign $\propto$ before a given parameter means that either the amplitude or the broadening of the peak is linked to that parameter.

Drude's model predicts monotonous decrease of $\varepsilon_r(\omega)$ for decreasing photon energy. It is also characterized by monotonous increase of $\varepsilon_i(\omega)$ (absorption tail) with decreasing photon energy towards the NIR region.



Starting values of a classical Drude function

Application to materials

This model fits well the optical properties of metallic samples and heavily doped semiconductors. The spectral range used for fitting depends on the material as shown in the array below.

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.

S.R. means Spectral Range.

Materials	$\varepsilon\infty$	ω_p	Γ_d	S. R. (eV)
Al	1.0	15.702	0.696	1.5 - 6.5
Co	3.694	12.175	5.799	0.75 - 4.75
Mo	-1.366*	19.972	8.357	1.5 - 5
NiCr	1.0	14.270	4.020	1.5 - 5
NiFe	1.0	14.790	4.780	1.5 - 5
Ti	1.0	10.9	2.53	1.0 - 6.0

References

1) J. M. Cazaux, *Introduction a la physique du Solide*, Masson (1996)
2) H. M. Rosenberg, *The Solid State*, Oxford University Press (1988)
3) F. Wooten, *Optical Properties of Solids*, Academic Press (1972)
4) E. Hecht, *Optics*, Chap. 3, Hardcover (2001)
5) www.ece.tamu.edu/People/bios/hemmer_files/15-dispersion.ppt

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