

Dispersion Model Basics

Optical constants define the interaction of light traveling through a material. As light passes into a new material, the optical constants determine the reflection from and transmission through the interface. In addition to intensity, the phase of each light beam can be calculated. Thus, an ellipsometry measurement can be “modeled” with knowledge of each layer thickness and corresponding optical constants. Figure 1 illustrates the interaction of light with a thin film on a substrate. If the film is transparent, the light will oscillate within the film and provide thickness information.

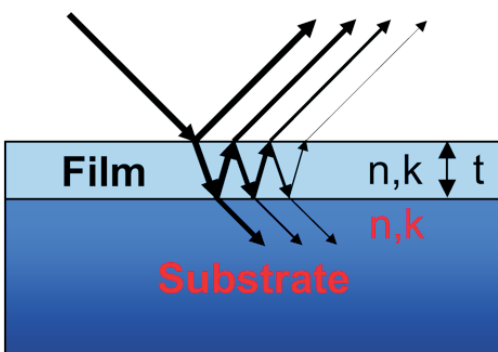


Figure 1: Interaction between light and thin film on substrate.

Optical constants are expressed as a complex number and can be separated into real and imaginary components. The most common representations are complex refractive index, \tilde{n} , and complex dielectric function, $\tilde{\epsilon}$. These two representations are related by:

$$\tilde{\epsilon} = \epsilon_1 + i\epsilon_2 = \tilde{n}^2 = (n + ik)^2$$

where ϵ_1 and ϵ_2 are the real and imaginary dielectric constants, respectively; and n and k are the index of refraction and extinction coefficient, respectively. Although the interaction of light with materials is described mathematically, the optical constants also provide some general insight. For instance, the index of refraction, n , relates the phase velocity, v , in a material to the speed of light in a vacuum, c , as:

$$n = \frac{c}{v}$$

The extinction coefficient, k , describes the absorption of light as it travels through the material. It is related to the absorption coefficient, α , of a material via,

$$\alpha = \frac{4\pi k}{\lambda}$$

The optical constants change values for each frequency of light. Thus, a complete material description must also involve the wavelength dependence, which is referred to as *dispersion*. The dispersion can be provided as a table of values at each wavelength. However, this requires a large number of values

when fitting a new material. More commonly, the optical constant shape is described using an equation (**dispersion relationship**). This reduces the number of parameters that describe a material over many wavelengths.

Common for transparent materials is the Cauchy relationship, given as:

$$n(\lambda) = A_n + \frac{B_n}{\lambda^2} + \frac{C_n}{\lambda^4}$$

where three terms describe the index of refraction over a range of wavelengths, λ . Restricting the Cauchy to a transparent wavelength region leads to applications involving dielectrics, organics, and semiconductors below their band gap. The Cauchy relationship is shown for two oxides and a nitride in Figure 2. All have different amplitudes, but notice that the index decreases for each as wavelengths get longer. This shape is required by all transparent materials, although the Cauchy does not prohibit an “unphysical” shape.

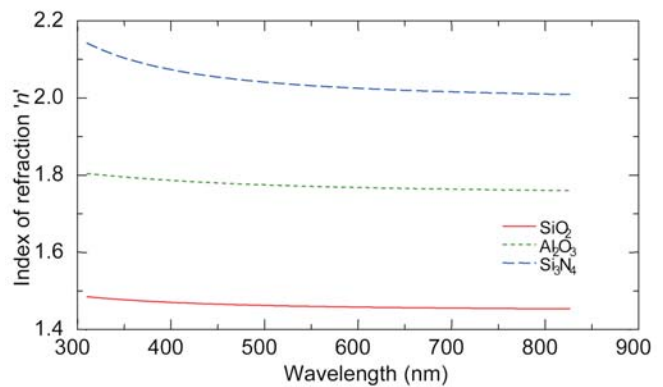


Figure 2: Cauchy dispersion for silicon dioxide, aluminum oxide, and silicon nitride.

The Sellmeier relationship is also appropriate for the transparent wavelength region. It will maintain a correct physical dispersion, as the index is determined from the enforcement of Kramers-Kronig (KK) consistency.

KK Consistency links the real and imaginary optical constants. In short, the shape of ϵ_1 (or n) depends on the shape of ϵ_2 (or k). When there is no absorption in the material, the index decreases toward longer wavelengths. This is referred to as normal dispersion. When absorption occurs, the index is also affected. If the absorption is strong, it will cause a change in direction for the real-component, which will return to normal dispersion after the absorption drops back down. The region of strong absorption is referred to as anomalous dispersion. This process is demonstrated in Figure 3 for absorption near 400 nm. The absorption causes ϵ_1 to change directions until the absorption decreases. The effect of absorption on ϵ_1 depends on the shape and amplitude of the absorption feature.

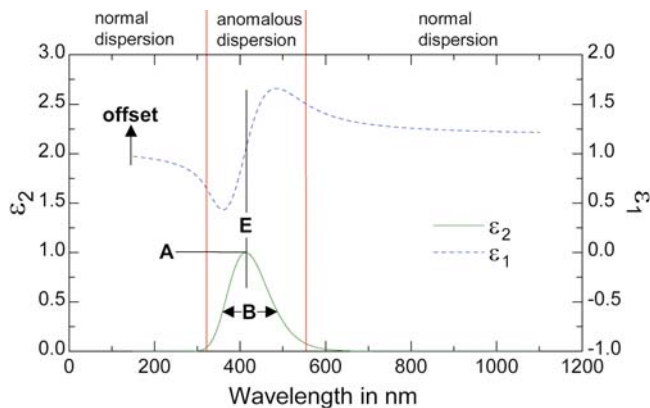


Figure 3: Dependence of both real and imaginary optical constants on an absorption feature modeled as an oscillator.

Oscillator models take advantage of the link between real and imaginary optical constants to describe the dispersion of materials in both absorbing and transparent region. By describing the absorption shape, they can use KK consistency to extract the shape of ϵ_1 . Many different oscillator models have been developed for this purpose: Lorentz, Gaussian, Harmonic, Tauc-Lorentz¹, Cody-Lorentz², and more. Each of these models mathematically describes the absorption feature using terms related to amplitude (A), broadening (B), and center energy (E). When KK consistency is used to determine the ϵ_1 shape, it can be shifted using an *offset* to correct for effects from absorption features beyond the measured spectral range. This is necessary because the KK transformation from ϵ_2 to ϵ_1 requires information about ϵ_2 at all wavelengths (not just those measured).

The absorption shape will depend on the source of that absorption. The most common features in the ultraviolet, visible, and infrared include electronic transitions, phonon absorptions, and free-carriers. Figure 4 shows the optical constants for a TiO₂ substrate versus photon energy measured with Spectroscopic Ellipsometry from the infrared to the vacuum ultraviolet³. The optical constants show absorption in both the ultraviolet and infrared regions. In the UV, the light is absorbed to provide energy to electronic transitions. This process excites an electron in the filled valence band of a material to an elevated state of the conduction band. The shape of the UV absorption will depend on the probability of electronic transitions at each energy (wavelength).

In the infrared, the absorption features are due to phonon absorption, as the slower frequencies are able to vibrate the much heavier atoms of the material. Free carrier absorption is not prominent in this graph of TiO₂, but can also occur in the infrared. This effect is more common for doped semiconductors, conductive dielectrics, and metals.

As evident from Figure 4, a real material is not necessarily

described by a single absorption oscillator. In practice, a series of oscillators can be summed together. The “Genosc” layer described in a previous Newsletter (Issue 2) allows the mixing of different types of oscillators to provide the best description of a material. For instance, a Drude oscillator can be used for free-carrier effects, while Lorentz oscillators describe the phonon absorption and a PSEMI-style oscillator describes the direct energy gap.

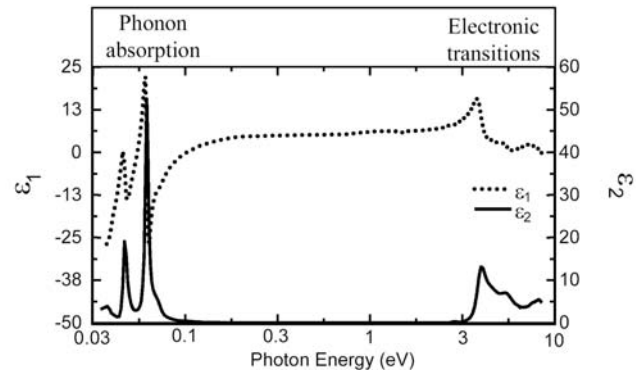


Figure 4: Optical Constants measured for TiO₂ [3].

This short discussion was taken from the JA Woollam Short Course lectures. More details can be obtained at these courses or from references 4 to 8.

References

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