

Sellmeier Dispersion by Dr. Tom Tiwald

If you have operated a spectroscopic ellipsometer, it is likely that you have also used the Cauchy dispersion layer. Its simplicity and convenience make it the most widely-utilized model for transparent materials. However, when the spectral range extends beyond the visible into the near-infrared, the refractive index of many transparent materials trend downward (as seen in Fig. 1). The Cauchy, which flattens at long wavelengths, cannot fit the near-IR index correctly.

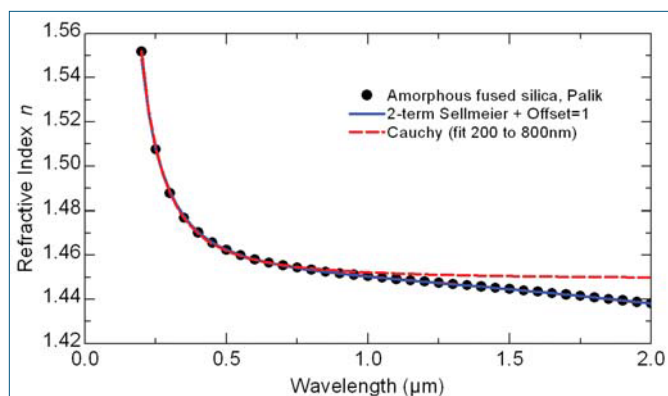


Figure 1. Sellmeier & Cauchy fits to amorphous fused silica from Palik².

Sellmeier¹ oscillators overcome this limitation. Figure 1, shows that a two-term Sellmeier equation clearly matches the near-IR index of SiO₂ (fused silica²) better than a three-term Cauchy. This is the result of the 2nd Sellmeier term “pulling” the index downward at long wavelengths.

Multiple-term Sellmeier equations are a more accurate representation of the index dispersion than the Cauchy. This is because the Sellmeier dispersion equation is the summation of zero-broadened Lorentz oscillators (see blue inset for details). This more closely matches the atomic theory of materials than the Cauchy equation, which is really just a Binomial series expansion of a single Sellmeier term. For common optical glasses, a three-term Sellmeier equation stays within 1×10⁻⁵ of the measured index over wavelengths from 365nm to 2.3μm³.

Visible-NIR Example: Ta₂O₅ Film

For comparison, we analyzed data acquired from a Ta₂O₅ film on silicon with both Cauchy and Sellmeier equations.

For wavelengths from 440-1000nm, both the Cauchy and Sellmeier models produce good fits (Fig. 2). The MSE and number of fit parameters (see table) are also comparable.

Wavelength Range	Cauchy $n = An + \frac{Bn}{\lambda^2} + \frac{Cn}{\lambda^4}$	Sellmeier $n^2 = 1 + \frac{(Amp1) \cdot \lambda^2}{\lambda^2 - (Wvl01)^2} + \frac{(Amp2) \cdot \lambda^2}{\lambda^2 - (Wvl02)^2}$
440-1000nm	MSE=3.02 # Index Fit Parms:3 (An, Bn, Cn)	MSE=3.09 # Index Parms: 2 (Amp1, Wvl01)
440-2066nm	MSE=5.9 # Index Fit Parms:3 (An, Bn, Cn)	MSE=3.07 # Index Fit Parms:3 (Amp1, Wvl01, Amp2), *Wvl02 is fixed at 20μm.

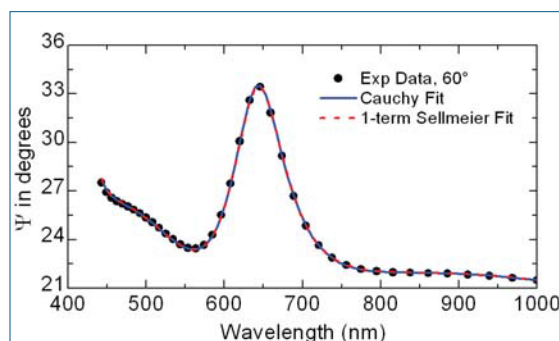


Figure 2. Fit to Ta₂O₅ film: 440 – 1000 nm.

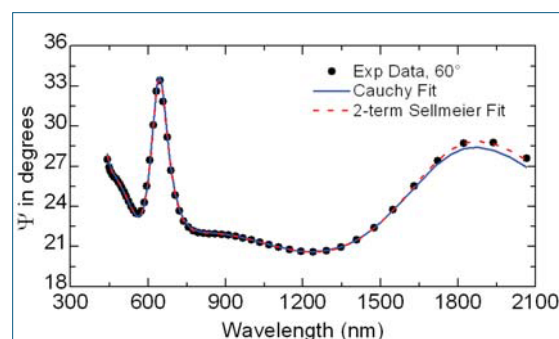


Figure 3. Fit to Ta₂O₅ film: 440 – 2066 nm.

When the spectral range is extended to 2.066 μm, the 2-term Sellmeier fit is significantly better than the Cauchy (Figure 3). The Sellmeier MSE = 3.07 is lower than the Cauchy MSE = 5.9 (see table). Thus, the Sellmeier is the model of choice when NIR wavelengths are measured.

The Sellmeier for mid-IR Wavelengths

The Sellmeier model is strongly recommended for the mid-IR wavelengths. Because many IR-transparent materials have strong vibrational absorptions at longer wavelengths, the Cauchy cannot accurately model the disper-

sion. A ZnSe example is shown in Figure 4. It should be noted that the strong “downturn” of the index at mid-infrared wavelengths is caused by infrared absorption that is outside of the wavelength range we are considering.

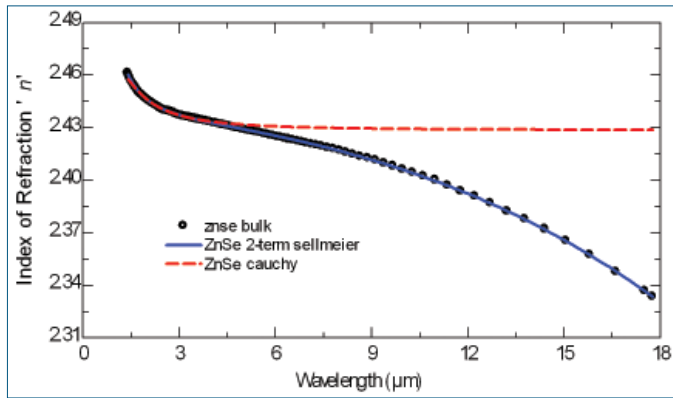


Figure 4. Sellmeier & Cauchy fits to ZnSe bulk sample.

Using the Sellmeier in WVASE32®

Sellmeier and Pole oscillators are available in the Genosc® layer. The available styles are described in the WVASE32® software manual Addendum.

GenOsc styles *Sell.2* and *Sell.7* (*Pole.2* and *Pole.7*) are equivalent to Eq. (1, 2) (blue inset), which is the most frequently cited Sellmeier form in the literature. To exactly match Eq. (1, 2), *e1_offset* must be set to 1.

The Sellmeier model can be implemented in the GenOsc layer in several ways. Figure 5 shows two sections used to access Sellmeier/Pole dispersion. The red box surrounds the built-in Poles that are always available in the GenOsc layer. The green box surrounds the oscillator list, where users have a choice of different Sellmeier and Pole types. Note the *e1_offset* (arrow) is added to either dispersion shape.

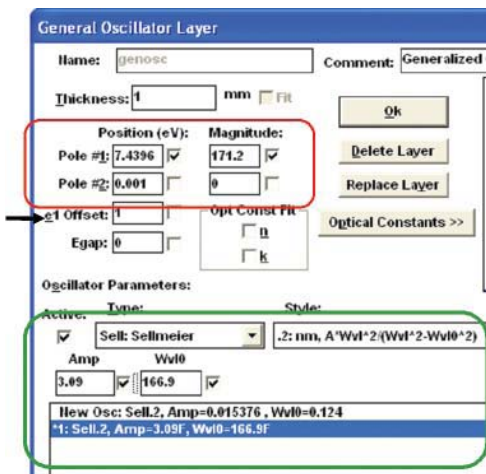


Figure 5. GenOsc with areas for the “built-in” Poles (red) and Sellmeier oscillator (in list) (green).

The Sellmeier Oscillator

In Sellmeier dispersion theory³, a material is treated as a collection of atoms whose negative electron clouds are displaced from the positive nucleus by the oscillating electric fields of the light beam (at IR wavelengths, the atoms themselves are displaced by the electric field). The oscillating dipoles resonate at a specific frequency (energy or wavelength), so the dielectric response is modeled as one or more Lorentz oscillators. Sellmeier theory assumes that the atomic dipoles have no absorption, so the broadening of the Lorentz oscillators equal zero. The resulting equations are usually written as:

$$\epsilon(\lambda) = n^2 = 1 + \sum_{k=1}^m \frac{A_k \cdot \lambda^2}{\lambda^2 - \lambda_k^2} \quad \text{Sellmeier} \quad (1)$$

or equivalently,

$$\epsilon(\lambda) = n^2 = 1 + \sum_{k=1}^m \frac{A_k}{E_n^2 - E^2} \quad \text{Pole} \quad (2)$$

Multiple terms are used for multiple resonances. Because there is no broadening term, the equations are purely real ($\epsilon_2 = k = 0$), and each term approaches $+\infty$ or $-\infty$ as λ approaches λ_k from the long or short wavelength sides, respectively. Thus a Sellmeier or Pole dispersion model *cannot* be valid in spectral ranges close to the resonant frequency. Figure 6 shows the $\text{Re}\{\epsilon\}$ for a two-term Sellmeier dispersion.

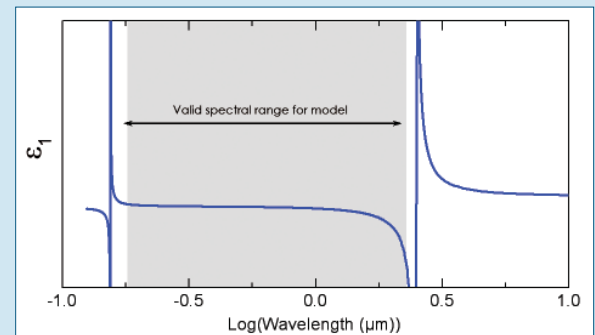


Figure 6. $\text{Re}\{\epsilon\}$, or ϵ_1 for a two-term Sellmeier.

References:

- ¹ L. Cauchy (Bull. des. sc. math, **14**, 9 (1830).
- ² Palik, Handbook of Opt. Constants I (pg. 753) & II (pg. 12).
- ³ W. Sellmeier, Annalen der Physik und Chemie **143**, 271 (1871).