

# The Gaussian Oscillator

By Tom Tiwald

For amorphous and glassy films, as well as some polycrystalline materials, absorption bands often have a Gaussian shape [1]. In these materials, atomic bond lengths and angles are randomly distributed around an average value. Therefore, each absorption band consists of numerous harmonic oscillators whose resonant frequencies have a normal distribution. The width of this distribution is orders of magnitude larger than the natural line width of the individual oscillators, therefore the absorption band has a Gaussian character.

These absorptions can be modeled using the Gaussian oscillator model found in the WVASE® *genosc.mat* and *user.mat* layers. The Gaussian oscillator equation (Genosc style *Gau.0*) is shown below and provides a shape as shown in Figure 1.

$$\epsilon_2(E) = Amp \cdot \left( e^{-\left(\frac{E-E_n}{\sigma}\right)^2} - e^{-\left(\frac{E+E_n}{\sigma}\right)^2} \right)$$

$$\epsilon_1 = \frac{2}{\pi} P \int_0^\infty \frac{\xi \epsilon_2(\xi)}{\xi^2 - E^2} d\xi$$

$$\sigma = \frac{Br}{2\sqrt{\ln(2)}}$$

Fit parameters are amplitude (*Amp*), center energy ( $E_n$ ) and broadening (*Br*) of the absorption peak. *Br* equals the Full-Width-Half-Maximum (FWHM) value.

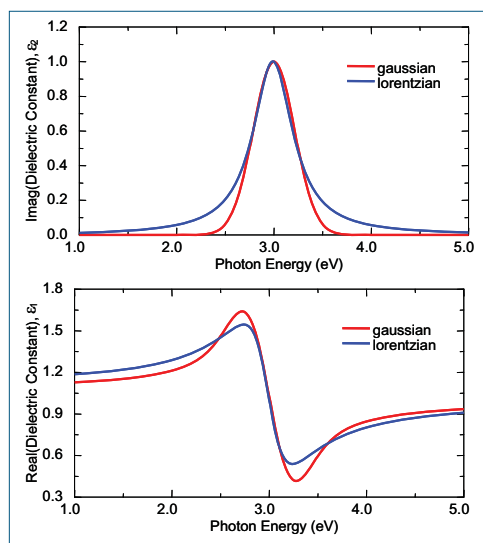


Figure 1. Comparison of Gaussian and Lorentz oscillators.

Note that the imaginary part of the dielectric function ( $\epsilon_2$ ) actually consists of a positive and negative energy Gaussian term. This makes  $\epsilon_2$  an odd function of photon energy ( $E$ ) – a necessary requirement for Kramers-Kronig consistency. The real part of the dielectric function,  $\epsilon_1$ , is given by the Kramers-Kronig transform of  $\epsilon_2$  (see ref. 1 for details).

## Applications

Beyond modeling glasses and other disordered materials, the Gaussian can be applied to many different types of materials. The primary advantage of the Gaussian is that  $\epsilon_2$  rapidly approaches zero beyond  $E_n \pm Br$ . This extremely useful characteristic makes the Gaussian an all-purpose oscillator that can model materials which are transparent over a limited portion of the measured spectral range. This behavior is quite different from the Lorentz oscillator, where  $\epsilon_2$  decreases slowly, as shown in Figure 1.

## Using Gaussian Oscillators

The Gaussian oscillator can be readily accessed from the Genosc® layer. The Gaussian oscillator type is first selected as the New Osc, then it is added via “Add Oscillator(s)” button or by holding Shift+Mouse click method (see the WVASE32 Addendum for further details). The fitable parameters, *Amp*,  $E_n$ , and *Br*, are easily adjusted using the mouse to drag the four “handles” (blue boxes, Figure 2, top), or typing a value into the variable (Figure 2, bottom).

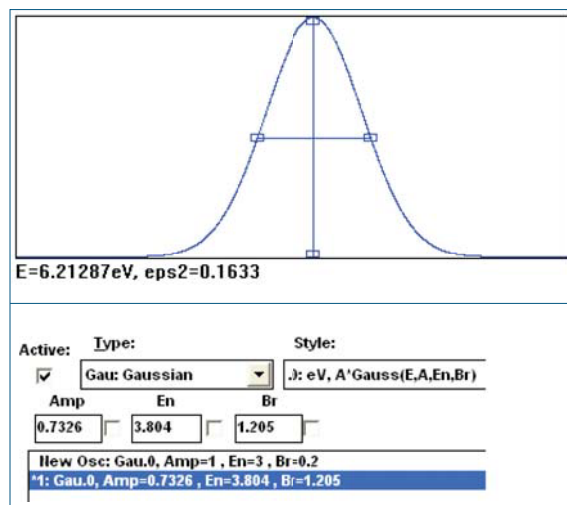


Figure 2. Gaussian oscillator in Genosc graph window (top) and as part of Genosc oscillator list.

### Example: Photoresist on Silicon

The first example is a polymer photoresist film on silicon. The reference dielectric function was obtained by:

1. Fitting film thickness and index in its transparent spectral range (600–1700nm) using a Cauchy model.
2. Fixing layer thickness and performing a point-by-point fit to all wavelengths (310–1700nm). Point-by-point fit values were saved as *resist1\_nk.mat*.

Next, the Cauchy layer was replaced with a Genosc® layer (same thickness), then:

3. *resist1\_nk.mat* was added as the reference material.
4. Six Gaussian oscillators were added and adjusted to fit the  $\epsilon_2$  function (see Figure 3).
5. The  $\epsilon_1$  reference dielectric function was fit by varying the Pole #1 Position and Magnitude.
6. The Genosc layer was closed, and all parameters (including thickness) were fit to the experimental ellipsometric  $\Psi$ - $\Delta$  data.

The resulting fit is shown in Figure 4, and the final Gaussian optical constants are shown in Figure 5.

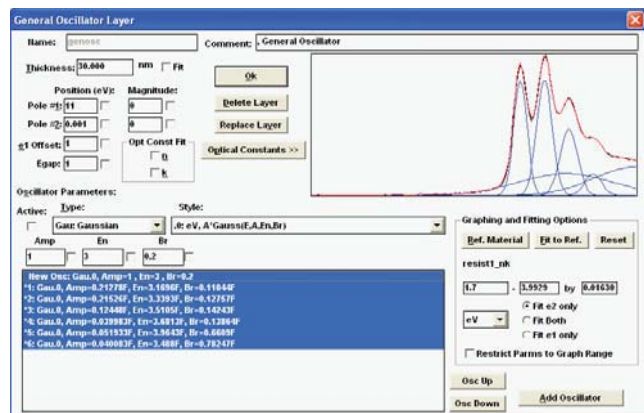


Figure 3.  $\epsilon_2$  of photoresist reference material fit with six Gaussian oscillators.

### Example: Float Glass (IR-VASE® data)

For mid-infrared dielectric functions of disordered materials, the Gaussian oscillator is generally superior to the Lorentz. This is illustrated in Figure 6, which compares Lorentz and Gaussian oscillator fits to an  $\epsilon_2$  spectra obtained from a bulk float glass sample. Here we show  $\epsilon_2$  for one of the Si-O absorption regions (850–1300  $\text{cm}^{-1}$ ).

Only four Gaussian oscillators are required to fit the absorption compared to 10 Lorentz oscillators. These results are typical for IR-VASE data obtained from glass and other amorphous materials.

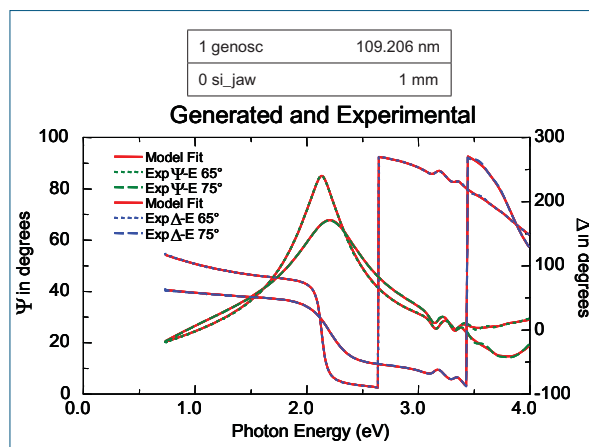


Figure 4. Resist on silicon Genosc Model and final  $\Psi$ - $\Delta$  experimental data fit.

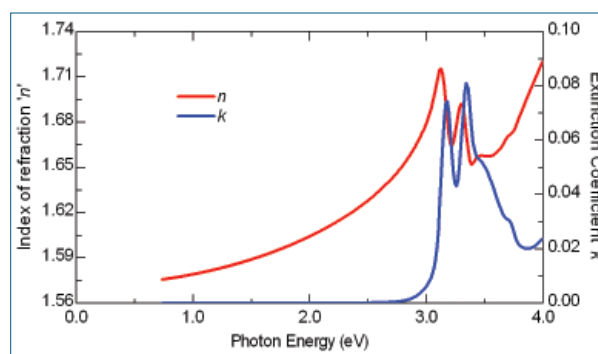


Figure 5.  $n(\lambda)$  &  $k(\lambda)$  for Gaussian oscillator model of photoresist layer.

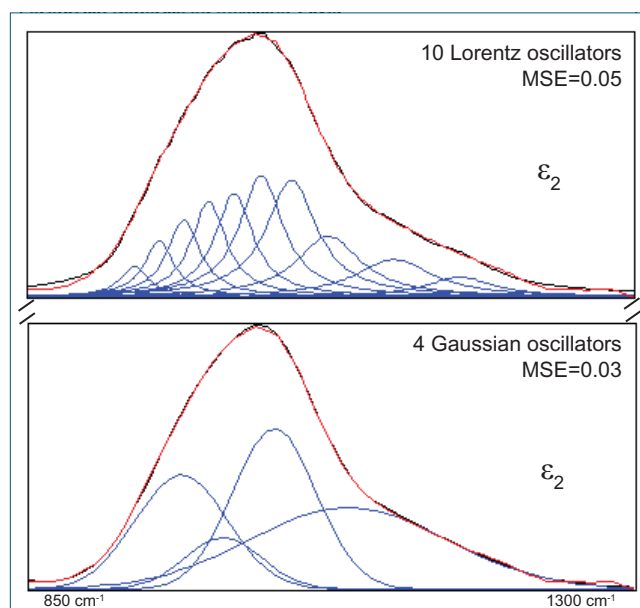


Figure 6. Top: 10-term Lorentz Oscillator fit to the Si-O vibration region for float glass. Bottom: 4-term Gaussian oscillator fit to the same region.

#### References:

1. D. De Sousa Meneses, M. Malki, & P. Echegut, *J. Non-Cryst. Solids* **351** (2006) 769.