

B-spline Dispersion Model in CompleteEASE[®]

For many years, the standard analysis approach for semi-absorbing films involved:

1. Cauchy dispersion to determine thickness from wavelength range where thin film is transparent.
 2. Fix thickness from #1 and fit “n,k” at all wavelengths.
- This procedure is often supplemented by:
3. Use “n,k” from #2 as reference for an oscillator model to fit data with smooth, Kramers-Kronig consistent curves.

Steps #1 and #2 are simple to apply. Step #2 is flexible and can match any features in the optical constant spectra. However, neither step enforces a physics-consistent (“physical”) shape to the resulting optical constants and can potentially produce incorrect results, e.g. discontinuities. Step #3 reduces the number of fit parameters, produces smooth spectral curves for “n,k” and enforces Kramers-Kronig consistency.

However, Step #3 is more complex. The user must choose the number and type of oscillators. For amorphous semiconductors and dielectrics, a single oscillator may match the optical functions from ultraviolet to near infrared. However, organic films, crystalline semiconductors, and metals may require 3-10 oscillators to cover this same spectral range.

The B-spline layer was developed in CompleteEASE as an alternative to the above approach - with the benefits of all steps. The B-spline can be thought of as a smooth, continuous, curve with:

- positive ϵ_2
- $\epsilon_2=0$ below bandgap, or over transparent wavelength range
- Kramers-Kronig consistent shape

The B-spline resolution can be adjusted to match optical constant features of any material. Consider a series of germanium thin films with varying crystallinity. The amorphous material absorption shape is very broad and fits a single Cody-Lorentz oscillator.

As the film becomes more crystalline, individual absorptions become more pronounced. These films would require multiple oscillators. A B-spline layer was used to fit all films in this series; including amorphous, nano-crystalline, micro-crystalline, poly-crystalline and single-crystal germa-

nium. The B-spline resolution was adjusted to ensure adequate resolution for all features in the optical spectra. A few optical functions from the B-spline fit are shown in Figure 1.

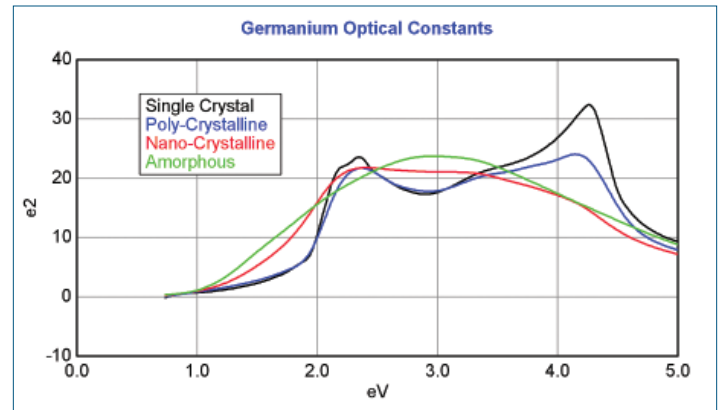


Figure 1. B-spline optical constants for a series of germanium thin films.

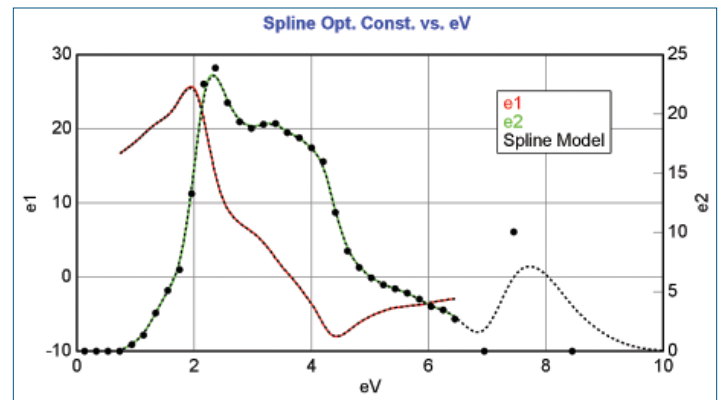


Figure 2. B-spline for micro-crystalline germanium film. The ϵ_2 spectra is defined by knots, whereas ϵ_1 is calculated from KK transform.

Figure 2 demonstrates the B-spline fit to a micro-crystalline germanium film. The ϵ_2 curve is defined by knots at 0.2eV intervals. It isn't necessary that the curve go through each knot due to the convex-hull property of the B-spline. However, the B-spline will maintain a smooth, continuous shape as a third order B-spline is continuous through the second derivative. Knots below the bandgap are forced to equal zero. The ϵ_1 spectra is calculated from a Kramers-Kronig transformation of the ϵ_2 spectra. As this KK integration requires information about ϵ_2 outside the measured spectra, there are extra knots at higher photon energy to guide the correct ϵ_1 shape. This is similar to the “poles” in the Gen-Osc layer.

In practice, data analysis with the B-spline is similar to the 3-step process described at the beginning of this article. If a

material is semi-transparent, a B-spline can be used to fit the transparent region (forcing $\epsilon_2 = 0$). After film thickness is determined, optical constants over the full spectral range are determined by fixing thickness and expanding the wavelength range (automatically in CompleteEASE with “Wavelength-Expansion” Fit). Finally, the resolution can be adjusted to ensure all features of the optical functions are adequately described. This is easier than with the GenOsc layer, as you can adjust the knot spacing and fit to see if the MSE lowers further. Eventually, all features will be adequately resolved and the MSE will show little change. This process was used to fit the data shown in Figure 3 measured from an organic film on silicon. With a knot spacing of 0.1eV, the optical features are well resolved, as shown in Figure 4. Again, this is a smooth, continuous, Kramers-Kronig consistent result with absorption equal to zero below the bandgap.

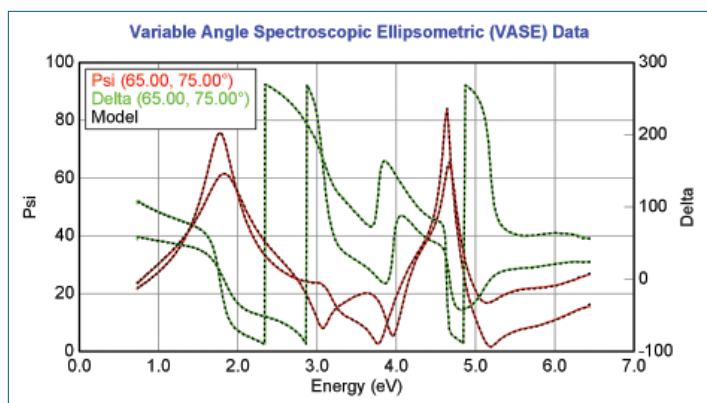


Figure 3. Data fit for an organic film on silicon.

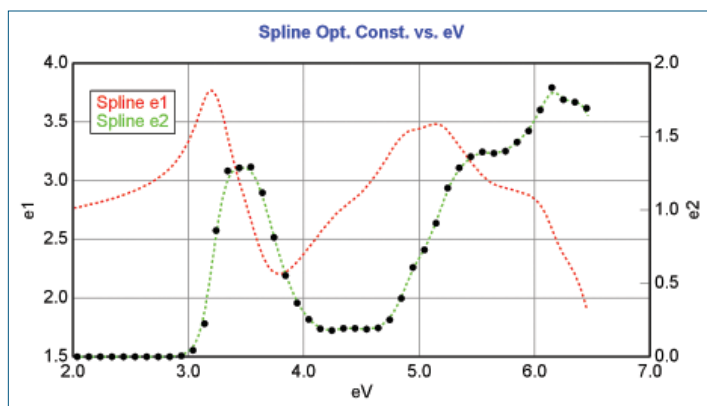


Figure 4. B-spline optical constants for the organic layer measured in Figure 3.

To reiterate the key advantages of the B-spline include:

- A. The B-spline is easier to apply than the Oscillator model, as it avoids most of the decisions related to oscillator type and number.
- B. The B-spline resolution can be adjusted to produce adequate resolution for any type of material - while minimizing the number of fit parameters.

- C. The B-spline can maintain Kramers-Kronig consistency, to ensure “physical” curve shapes. This reduces the number of parameters, as only one curve is described, while the other gets its shape from KK consistency.

Future of B-spline:

To further reduce the number of fit parameters, it is beneficial for many materials to customize the knot resolution versus wavelength. For example, direct-gap semiconductors will require fine-resolution at the bandgap, but this resolution may not be required elsewhere. Figure 5 shows experimental data for a GaN coating on SiC substrate. The data are fit well with a variable-knot spacing, as shown in Figure 6, with 0.02eV resolution near the bandgap and 0.4eV resolution at both higher and lower photon energies. Custom knot spacing was recently added to the B-spline layer and may prove to be very valuable for a host of different material problems.

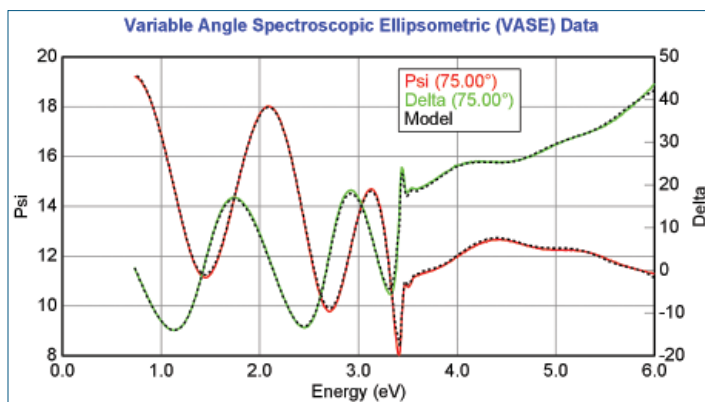


Figure 5. Data fit for a GaN film on SiC.

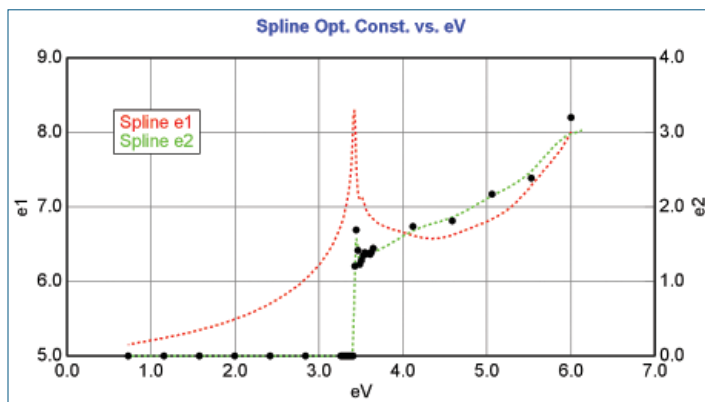


Figure 6. Variable B-spline node spacing provides enhanced resolution near the bandgap.

For more technical details regarding the b-spline, please refer to: B. Johs and J.S. Hale, “Dielectric function representation by B-Splines” *Phys. Stat. Sol. (a)*, **205**, No. 4, (2008) 715-719.