Common Questions about Anisotropy

by James Hilfiker

Anisotropic samples provide exciting new challenges to ellipsometry researchers. Advanced measurements and data analysis techniques are now available to enable anisotropic characterization. However, these techniques are seldom 'push-button' and require an understanding of the primary issues. Hopefully, the following discussions will move you toward that understanding.

Q: What is anisotropy?
A: In a normal "isotropic" sample, the optical properties are the same in all directions. Anisotropy refers to the directional-dependent optical properties of a material. In other words, the *n,k* values may be different for electric fields (light) traveling through the material in different directions. Figure 1 show the ordinary and extraordinary optical constants of 4H silicon carbide.

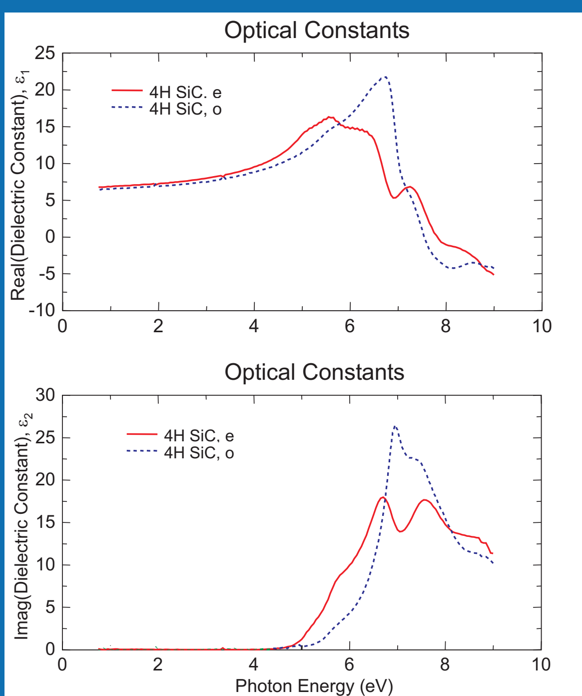

Figure 1. Anisotropic crystalline SiC optical constants.

Q: What do Uniaxial and Biaxial refer to?
A: A uniaxial material has 2 different optical properties ($n_x = n_y \neq n_z$). A biaxial material has 3 different optical constants ($n_x \neq n_y \neq N_z$).

Q: Why is a material anisotropic?
A: The optical properties of a material depend on the underlying atomic or molecular structure. If this basic building block has a non-symmetric 'shape' and a long-range order throughout the material, then the material can be anisotropic. For example, an electronic transition may occur at different resonant energies depending on the spacing between atoms in a non-cubic crystal. This would lead to different *n,k* values across the spectrum.

Q: What are common anisotropic materials?
A: Due to the need for both non-symmetric "shape" and long-range order, anisotropic materials tend to be of a couple types: non-cubic crystals and ordered organics. Included in the first type are such materials as rutile (with tetragonal symmetry) and sapphire with its hexagonal crystal structure. A few anisotropic organics include liquid crystal films and PET.

Q: ***What special methods can be applied when measuring anisotropic materials?***
A: This is a very open question, as it depends on the type of anisotropy (uniaxial, biaxial), the type of sample (substrate only, thin film, transparent or opaque substrate,…), and the orientation of the anisotropic material. For many simple samples, the anisotropic orientation is aligned with the sample normal ($n_x = n_y \neq n_z$). For this case, it is best to measure a wide range of incident angles to change the path length the light travels through the film (experiencing different optical properties in different directions as it goes). This type of anisotropy can be handled without resorting to *Generalized Ellipsometry*.

Q: What is Generalized Ellipsometry?
A: This refers to an advanced ellipsometry measurement that involves the complete 2X2 Jones matrix description of the sample. Normal ellipsometry ignores the off-diagonal elements of this matrix, as they are zero for isotropic materials. Equation 1 below is the Jones matrix for an isotropic sample. Anisotropic materials can cross-couple the p- and s- polarized light, leading to non-zero off diagonal elements. To get the full details of the 2X2 Jones matrix, requires 6 values (3 Psi and 3 Delta) instead of the standard 2 terms (Psi and Delta) of a normal ellipsometry measurement. Equation 2a gives the Jones matrix representation for an anisotropic sample. Equations 2b-2d are our definitions of the measured generalized ellipsometry parameters.

$$\begin{pmatrix} E_p^{out} \\ E_s^{out} \end{pmatrix} = \mathbf{J} \begin{pmatrix} E_p^{in} \\ E_s^{in} \end{pmatrix} = \begin{pmatrix} r_{pp} & 0 \\ 0 & r_{ss} \end{pmatrix} \begin{pmatrix} E_p^{in} \\ E_s^{in} \end{pmatrix} \qquad (1)$$

$$\begin{pmatrix} E_p^{out} \\ E_s^{out} \end{pmatrix} = \begin{pmatrix} r_{pp} & r_{sp} \\ r_{ps} & r_{ss} \end{pmatrix} \cdot \begin{pmatrix} E_p^{in} \\ E_s^{in} \end{pmatrix} \qquad (2a)$$

$$AnE = \tan(\Psi) \cdot e^{i\Delta} = \frac{r_{pp}}{r_{ss}} \quad (2b)$$

$$Aps = \tan(\Psi_{ps}) \cdot e^{i\Delta_{ps}} = \frac{r_{ps}}{r_{pp}} \quad (2c)$$

$$Asp = \tan(\Psi_{sp}) \cdot e^{i\Delta_{sp}} = \frac{r_{sp}}{r_{ss}} \quad (2d)$$

Q: If I don't use Generalized Ellipsometry, am I ignoring the sample anisotropy?
A: No, the standard Psi and Delta data will be affected by the anisotropy, but there won't be enough information to determine how they were affected. The off-diagonal elements are needed to help distinguish how the standard data were affected by anisotropy.

Q: How do I handle anisotropic substrates?
A: This question depends on the information you are searching to find. Are you interested in (i) the substrate material properties? Or (ii) measuring films on this anisotropic substrate?
(i) If you are interested in the substrate material properties, which will be directional dependent, you are best served by a series of *generalized ellipsometry* measurements at different incident angles and possibly at different sample orientations. It is probably best to discuss your application with a Woollam Applications engineer as they can provide great input into the best approach for each type of substrate.
(ii) If you don't care about the substrate, but need to measure thin films on this surface, you have a couple of options. First, you can roughen the back of transparent substrates. The anisotropy effects are strongest after traveling through a substrate and returning to the surface. If this "backside" reflection can be avoided (by scattering the light of the back surface or spatially separating this secondary beam), the substrate anisotropy effects will be minimal. Second, you can work through the full characterization of a bare substrate and then use this in your model for the coated samples. However, this is much more time consuming.

Q: How do I model anisotropic materials?
A: The Woollam analysis software uses a layer called "biaxial.mat" to describe up to 3 orthogonal optical properties. The orientation of these three values can be adjusted via three Euler angles. These three angles rotate and tilt the optical axes to correct for the true position of the material properties relative to the ellipsometer sample position.

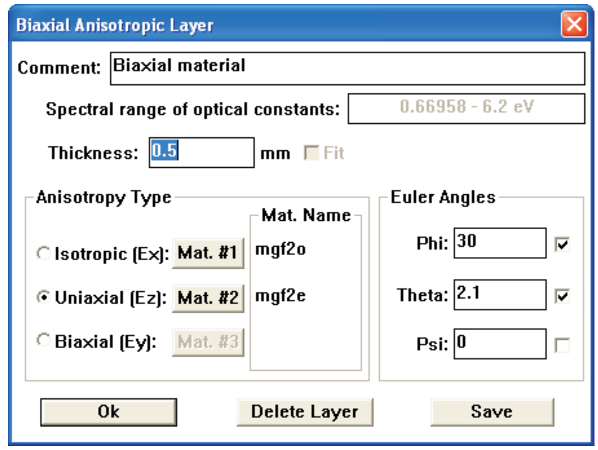

Figure 2. Biaxial.mat layer for describing the optical properties of an anisotropic material.

Q: How do I adjust the Euler angles?
A: There is a nice description of the Euler angles in the WVASE32 addendum. However, it is best to get started with a few simple facts. First, it unlikely you will need all three angles. For simplicity, try to describe the material with the first 2 Euler angles (Phi and Theta). Phi rotates the in-plane orientation around the sample normal. Theta will tip the Z-direction away from the sample normal. There are examples using different Euler angles in the WVASE32 addendum.

Q: How sensitive is ellipsometry to the anisotropy in a material?
A: This question depends on the path length in the material. For substrates, transmission ellipsometry can be sensitive to Δn of 0.00001 or smaller. However, a 10nm thick film will show sensitivity to Δn about 0.1.

Q: Where can I find out more about anisotropy?
A: Most of the software-related information is handled by the WVASE32 addendum, with sections describing "anisotropic" data acquisition, the biaxial layer, Euler angles, and general anisotropic sample procedures.

An excellent resource for generalized ellipsometry comes from Mathias Schubert's chapter in the Handbook of Ellipsometry, features on Page 10. Dr. Schubert has published dozens of papers on the theory and application of generalized ellipsometry and this chapter is a nice review from the world-expert.