# Appendix A: Basic Ellipsometry

A-1
Ellipsometry Introduction

Ellipsometry uses polarized light to characterize thin film and bulk materials. A change in polarization is measured after reflecting light from the surface. Thin film thickness (t) and optical constants (n, k) are derived from the measurement. Information is obtained from each layer interacting with the measure-ment. Light returning from the film–substrate interface interferes with the surface reflection to provide layer information (figure to right).

1. Known input polarization

3. Measure output polarization

2. Reflect off sample ...
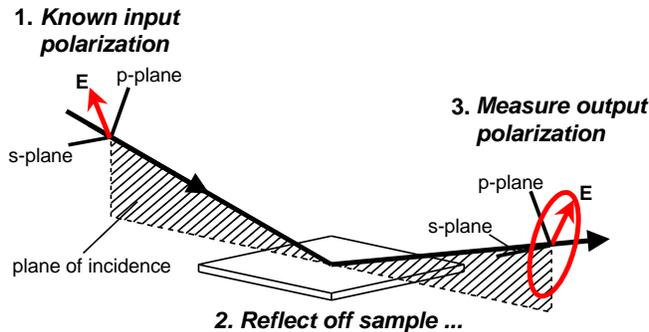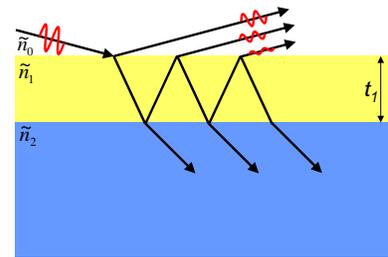
An ellipsometry measurement is a description of the change in polarization (figure to left) as polarized light is reflected from a sample surface. It is expressed as two parameters for each wavelength-angle combination: Psi (ψ) and Delta (Δ). These values can be related to the ratio of complex Fresnel reflection coefficients, r_p and r_s, for p- and s- polarized light, respectively.

$$\rho = \frac{r_P}{r_S} = \tan(\psi)e^{i\Delta}$$

Ellipsometry offers three main advantages over simple intensity-based reflection or transmission measurements:

1. Measurement is defined by a ratio, thus ellipsometry is not sensitive to changes in absolute intensity of measurement beam (i.e. the sample becomes the 'reference' for the measurement).
2. Phase information (from Δ) provides enhanced sensitivity to ultra-thin films, even down to sub-nm level.
3. Ellipsometry measures 2 values (Ψ and Δ) at each wavelength, doubling the information content compared to an intensity reflection or transmission measurement.

For further reading:

1. H. Fujiwara, *Spectroscopic Ellipsometry Principles and Applications*, West Sussex, John Wiley & Sons, 2007.
2. H.G. Tompkins and W. A. McGahan, *Spectroscopic Ellipsometry and Reflectometry*, New York: Wiley, 1999.
3. H.G. Tompkins and E.A. Irene (eds), *Handbook of Ellipsometry*, New York: William Andrew, 2005.

A-2
Data Analysis Overview

Data analysis is a very important part of spectroscopic ellipsometry (SE): without data analysis, SE only measures the ellipsometry parameters Psi and Delta versus wavelength.

Data analysis is used to determine optical constants, layer thickness, and other material properties. The basic steps of this approach include:

1. SE data is measured on the sample.
2. A model describes the measured sample using layers for each material. Thickness and optical constants (n and k) describe each layer over the measured wavelength range, with estimates for any unknown properties.
3. The unknown properties of the sample are defined as model "fit" parameters. The software automatically adjusts these parameters to improve the agreement between the measured and model-generated data.
4. The results of the fit are evaluated. If results are not acceptable, the process can be repeated with a new model or different "fit" parameters until the best description is found.
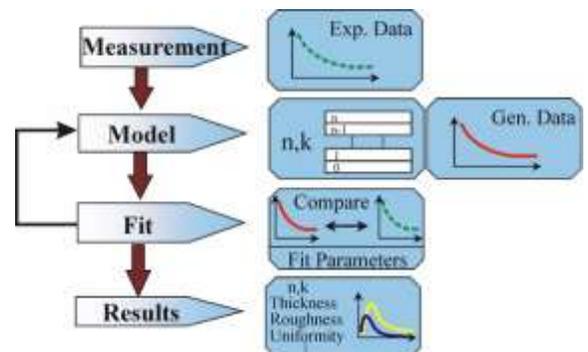

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Optical constants of isotropic materials can be described using two parameters. These values characterize how a material responds to excitation by light of a given wavelength. One representation is the complex index of refraction, $\tilde{n}$, where the real part n is the index and the imaginary part, k, is the extinction coefficient.

$$\tilde{n} = n + i\mathrm{k}$$

The index, n, describes phase velocity of light in a material compared to propagation in vacuum. The figure to right shows light traveling through different media, where the index of air, Film 1, and Film 2 is n=1, 4, and 2, respectively. Film 1 is also absorbing, as demonstrated by the exponential decrease in amplitude as the film travels through. The absorption of light is governed by the extinction coefficient, k. These quantities also determine the amount of light reflected and transmitted at an interface between two materials. A large index difference will reflect more light at the interface.
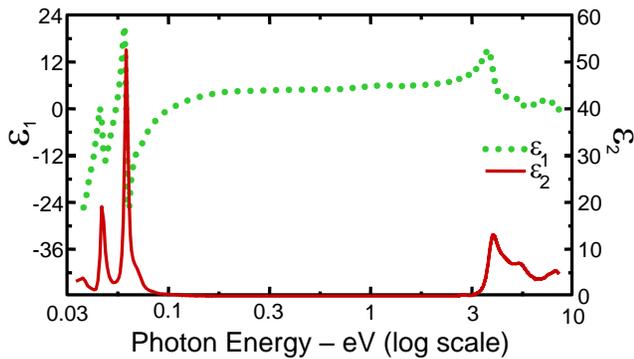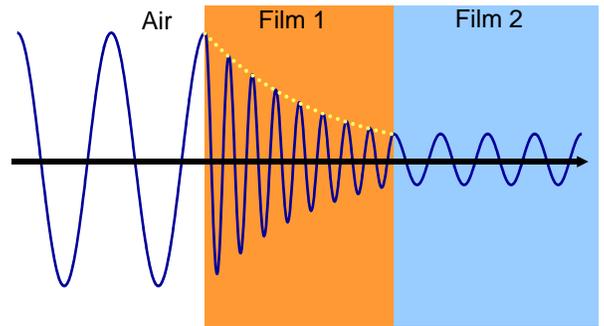
Alternately, the optical constants can be described using the complex dielectric constant, given as $\tilde{\varepsilon}$. The complex dielectric constant is related to the complex index of refraction by:

$$\tilde{\varepsilon} = \tilde{n}^2$$

Both are commonly encountered in the literature.

The optical constants will vary at different wavelengths, as shown for TiO_2 in the Figure to left. The absorption, given by ε_2, will occur due to different mechanisms in the material, such as phonon vibration or electronic transitions.

Appendix B: Measurement Details

B-1
Standard Spectroscopic Ellipsometry

Traditional ellipsometry measures the relative change in polarization due to reflection/transmission from a sample as,

$$\rho = \frac{r_P}{r_S} = \tan(\psi)e^{i\Delta}$$

where the sample is described using only the diagonal elements of a 2 X 2 Jones matrix.

$$\begin{pmatrix} E_p \\ E_s \end{pmatrix}_{out} = \begin{bmatrix} r_p & 0 \\ 0 & r_s \end{bmatrix} \begin{pmatrix} E_p \\ E_s \end{pmatrix}_{in}$$

This definition is valid for isotropic samples and certain orientations of uniaxial anisotropy. Thus, a standard ellipsometry measurement does not involve any cross-coupling between p- and s- polarization directions. The amplitude ratio, tan(Ψ) and the relative phase difference, Δ, are measured by comparing the effects of light in p- and s- directions respectively. In this manner, the measurement is self-referencing and can be highly accurate.

B-2
Intensity Measurements

In addition to ellipsometry measurements, which measure the polarization change, most ellipsometers can also collect intensity-based (spectrophotometric) measurements. This can include polarized or cross-polarized reflectance and transmittance data. As these measurements require accurate intensity values, they are generally less accurate than ellipsometry measurements, which are self-referencing. The tangent of Psi is related to the amplitude ratio of Fresnel reflection or transmission coefficients. These are in-turn equal to the square root of the Reflectance (R) or Transmittance (T) intensity measurements.
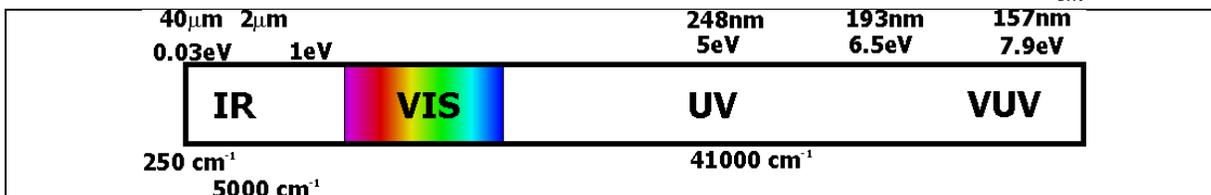
$$\tan(\psi) = \frac{|r_P|}{|r_S|} = \frac{\sqrt{R_P}}{\sqrt{R_S}}$$

B-3
Wavelength Units

Light can be described in various units: wavelength (λ), photon energy (E), and wavenumber (K). Wavelength is the distance between adjacent peaks of an electromagnetic wave, commonly given in nanometers (nm) or microns (μm). Wavenumber refers to the number of waves in a length of one centimeter, with units of reciprocal centimeters (cm^{-1}).

If light is treated as a quantum of radiant energy (photon), its energy is given in electron volts (eV) which is proportional to frequency. Choice of units depends largely on the spectral range and application. The following figure illustrates the full spectral capability of Woollam ellipsometers with representative wavelengths, photon energies, and wavenumber across the infrared (IR), visible (VIS), ultraviolet (UV), and vacuum ultraviolet (VUV). The following relationships convert between various units:

$$\lambda_{nm} = \lambda_{\mu m} \times 1000 \qquad \lambda_{nm} = \frac{1240}{E_{eV}} \qquad \lambda_{\mu m} = \frac{10,000}{K_{cm^{-1}}}$$

40μm 2μm			248nm	193nm	157nm
0.03eV 1eV			5eV	6.5eV	7.9eV
IR	VIS	UV			VUV
250 cm^{-1}		41000 cm^{-1}			
5000 cm^{-1}					

Ellipsometry measurements are acquired at oblique angles of incidence, with typical angles between between 45° and 80° relative to the sample normal. At these angles, there is high sensitivity to the differentiation between p- and s- polarized light. If polarized light reflects from an isotropic material, the s-polarized light will increase with angle of incidence, while the p-polarized light goes through a minimum at the Brewster angle before climbing back up.

This is shown in the following figure for a coated glass slide. The reflected intensities are shown for both p- and s- polarized light. The ellipsometry parameters (Ψ and Δ) are defined from the complex ratio of Rp and Rs given the values shown in the corresponding figure. Notice, the largest changes occur at oblique angles (in this case near 65°).
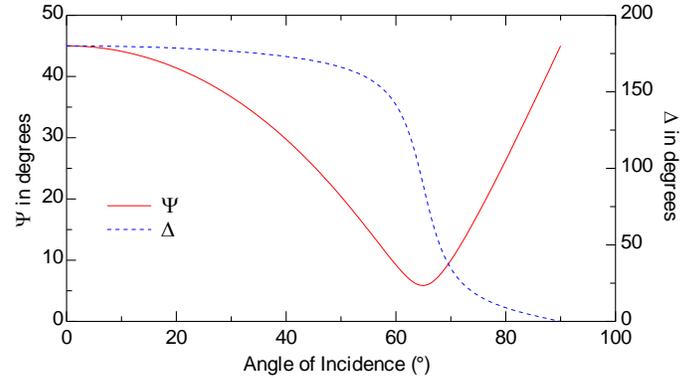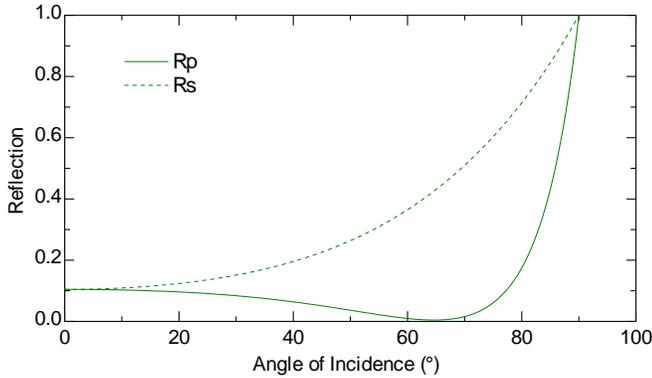
NOTE: With modern ellipsometers, it is not critical to measure at the Brewster angle. All Woollam ellipsometers include a compensator (see B-6), which allows precise measurements over a wide range of angles. However, the change in polarization would be negligible at angles near normal incidence. Thus, it is still important to use oblique angles for common SE applications.

B-5
Spectroscopic Ellipsometry or Single-wavelength?

A single wavelength ellipsometer measures two pieces of information that describe amplitude and phase changes due to the sample (Ψ and Δ) for that single wavelength. This information can be used to determine a maximum of 2 unknown sample properties: n and k of a bare substrate; n and t for a transparent film on known substrate, etc. Spectroscopic ellipsometry measures 2 values at every wavelength. Thus, with 100 measured wavelengths, there are 200 data points. All of this information can be used to solve material questions.

Even in the simple case of a transparent layer on known substrate, this is equivalent to using 100 separate single-wavelength ellipsometers to get the one unique answer. However, the benefits are far more reaching, because each wavelength probes the same sample with different light frequency. If one wavelength is insensitive to the film because of poor data response, the other 99 wavelengths can help insure a correct response. In addition to possible insensitive regions, the measurement from a single-wavelength will repeat itself (for transparent film). This introduces multiple solutions for the exact same data point (see figure below- left). This problem is solved with spectroscopic measurements. Even though the data at one wavelength may match for various possible solutions, the surrounding wavelength data will uniquely determine the correct answer (see figure below-right).
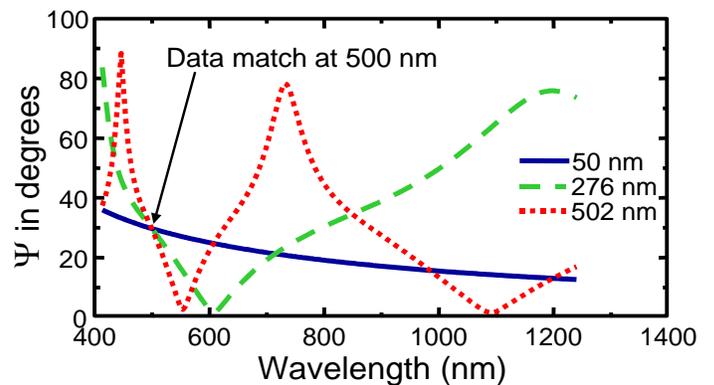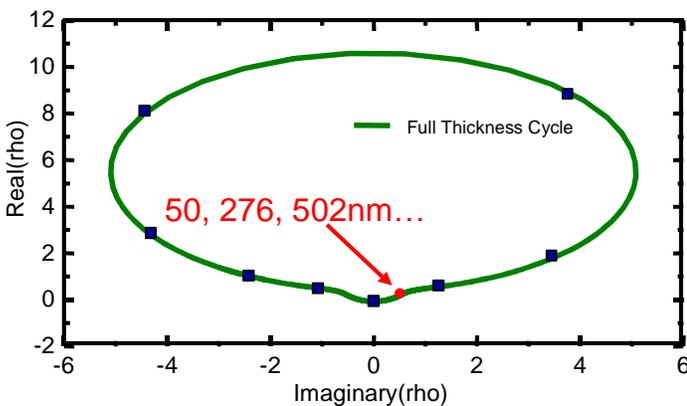
B-6
Ellipsometry with an adjustable Retarder or Compensator

Many ellipsometer types utilize polarizers for their measurement: rotating analyzer (RAE) and Rotating Polarizer (RPE) in particular. These ellipsometers are very simple to construct and can be very accurate. However, they have known limitations:

1. Can't determine the 'handedness' of Δ
   (Δ can range from 0 – 360°, but an RAE or RPE mirror all D values to 0-180°)
2. Precision and accuracy of measured Δ is poor when Δ is near 0° or 180°.

These limitations are inconsequential for many applications, but limit the accurate measurement of some difficult samples. We eliminate these problems by simply adding a compensator to the beam path (either before or after the sample). Our standard instruments all incorporate patented compensator technology to acquire the highest accuracy measurements.

> VASE and VUV-VASE: RAE with AutoRetarder
> M-2000, alpha-SE and IR-VASE: Rotating Compensator Ellipsometer (RCE)

In addition to highly accurate Δ measurements over the full 0-360° range, an adjustable or rotating compensator also enables measurements of depolarization (see Appendix B-7).

B-7
Depolarization

Ellipsometry measurements use polarized light. If the sample is isotropic and ideal, this measurement can be described by two parameters: ψ and Δ. However, if a sample is partially depolarizing, two parameters are insufficient to fully describe the ellipsometry measurement. The addition of an adjustable or rotating compensator (See B-6) permits separate measurements of three quantities, reported as: ψ, Δ, and *%depolarization*.

Depolarization of the light beam can occur with nonuniform layer thicknesses, patterned films, finite spectral bandwidth, finite angular bandwidth, and backside effects from transparent substrates (see B-8). Fortunately, the effects of these non-idealities on standard ellipsometry data can be quantified by measuring (and modeling) the depolarization. This allows separation of the non-idealities from thin film model to insure the correct thickness and optical constants are determined.

B-8
Transparent Substrates

Ellipsometry measurements are commonly taken on transparent substrates. In this case, the light reaching the detector may include reflections from the back-side of the substrate (bottom left figure). Substrates are generally thicker than the coherence length for the light source of the ellipsometer. Thus, the returning light does not interfere in a coherent sense, as its phase information is lost compared to the reflections from the top-surface coatings.

This "incoherent" summation of light beams can be handled mathematically. In addition, there is generally some depolarization of the measurement. If the depolarization is measured (see B-7), the amount of light returning from the back-side is easily quantified.

Back-side reflections are typically undesirable when characterizing surface films. This is especially true if the substrate is anisotropic. To prevent back-side reflections the surface can be roughened to scatter light (bottom right figure). In other cases, translucent tape applied to the backside of substrate is adequate to suppress the backside reflections*.
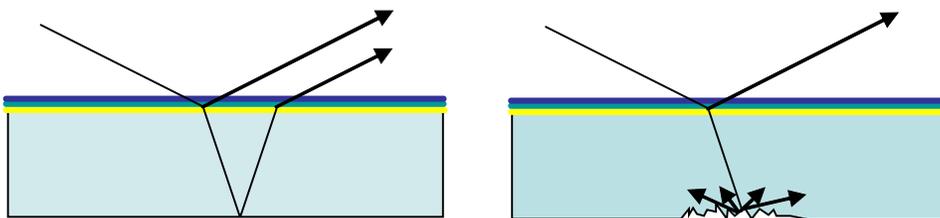
*R.A. Synowicki, "Suppression of backside reflections from transparent substrates", Phys. Stat. Sol. (c) 5, (2008) 1085-1088.

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B-9
Generalized Ellipsometry

Generalized ellipsometry involves all four components of the Jones matrix. With this description of the sample, the experimental data are presented as three sets of ψ, Δ pairs

$$\begin{pmatrix} E_p \\ E_s \end{pmatrix}_{out} = \begin{bmatrix} R_{pp} & R_{sp} \\ R_{ps} & R_{ss} \end{bmatrix} \begin{pmatrix} E_p \\ E_s \end{pmatrix}_{in}$$

AnE

$$\rho = \frac{R_{pp}}{R_{ss}} = \tan(\psi)e^{i\Delta}$$

Aps

$$\rho_{ps} = \frac{R_{ps}}{R_{pp}} = \tan(\psi_{ps})e^{i\Delta_{ps}}$$

Asp

$$\rho_{sp} = \frac{R_{sp}}{R_{ss}} = \tan(\psi_{sp})e^{i\Delta_{sp}}$$

The off-diagonal elements of the Jones matrix (Rsp and Rps) will be zero for isotropic samples and special orientations of anisotropic samples. Thus, generalized ellipsometry is typically used for the characterization of anisotropic materials.

B-10
Retardation Measurements

Ellipsometers measure the phase change of light. For retardance measurements, light transmits through the substrate, as shown in the figure below. Two orthogonal waves enter the birefringent material in-phase. A phase change, δ, is induced by the material as the index of refraction (and thus phase velocity) differs along the fast- and slow-axis. Generalized ellipsometry measurements (see B-9) can determine the fast-axis orientation and provide a correct measure of retardance.
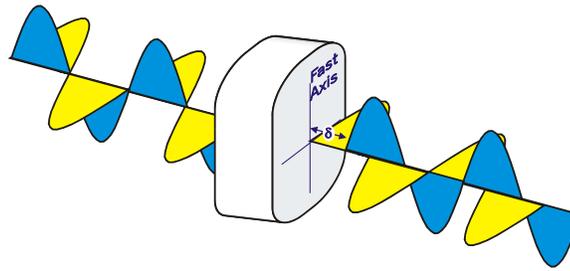
B-11
Mueller-matrix Ellipsometry

Standard ellipsometry measurements assume 1) the measurement beam remains 100% polarized and 2) the off-diagonal elements are zero (no cross-coupling between p- and s-polarizations). These assumptions are appropriate for a large variety of materials characterization problems. If assumption 1 is not valid, it is often possible to use an advanced ellipsometer design and measure the amount of depolarization (Appendix B-7). If the sample is anisotropic, assumption 2 may not be valid, which often requires generalized ellipsometry measurements (See Appendix B-9). In the rare case where both assumptions fail at the same time (i.e. the sample is both depolarizing and anisotropic), the more general Mueller-matrix measurement is necessary.

Mueller-matrix ellipsometry replaces the standard 2x2 Jones matrix description of the sample with a more general 4x4 matrix. The Mueller-matrix maps the Stokes parameters for incoming to outgoing light, using the following notation.

$$\begin{bmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{bmatrix}_{OUT} = \begin{bmatrix} M_{11} & M_{12} & M_{13} & M_{14} \\ M_{21} & M_{22} & M_{23} & M_{24} \\ M_{31} & M_{32} & M_{33} & M_{34} \\ M_{41} & M_{42} & M_{43} & M_{44} \end{bmatrix} \cdot \begin{bmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{bmatrix}_{IN}$$

To determine all 16 elements of the Mueller-matrix would require a compensator before and after the sample. Fortunately, there is often symmetry within the Mueller-matrix elements that allows a complete characterization of difficult samples without measurement of all 16 elements.

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Appendix C: Modeling and Data Analysis

C-1
Modeling Overview

As described in Appendix A-3, it is important to analyze the data (Ψ and Δ) to determine optical constants, layer thickness, and other material properties.

A model describes the measured sample using layers for each material. Thickness and optical constants (*n* and *k*) describe each layer over the measured wavelength range, with estimates for any unknown properties. An example model is shown below with a silicon substrate (layer 0) and two coatings above (layer 1 and 2).

The unknown properties of the sample are defined as model "fit" parameters. The software automatically adjusts these parameters to improve the agreement between the measured and model-generated data. This agreement is quantified via the Mean Squared Error (See Appendix C-2).

| 2 ta2o5	200 nm
1 sio2	20 nm
0 si	1 mm

C-2
Mean Squared Error

The MSE describes the difference between experimental data and model predicted data:

$$MSE = \frac{1}{2N-M} \sum_{i=1}^{N} \left[\left(\frac{\psi_i^{mod} - \psi_i^{exp}}{\sigma_{\psi,i}^{exp}} \right)^2 + \left(\frac{\Delta_i^{mod} - \Delta_i^{exp}}{\sigma_{\Delta,i}^{exp}} \right)^2 \right] = \frac{1}{2N-M} \chi^2$$

The subscript "*i*" identifies each unique wavelength and angle of incidence, σ is the standard deviation, *N* is the total number of (ψ, Δ) pairs, M is the number of "fit parameters", and "exp" and "mod" signify experimental and calculated values. Another common estimator, chi-square (χ^2), is also defined.

The MSE compares the merit of different models to help find a physical sample description that best matches the experimental measurement.
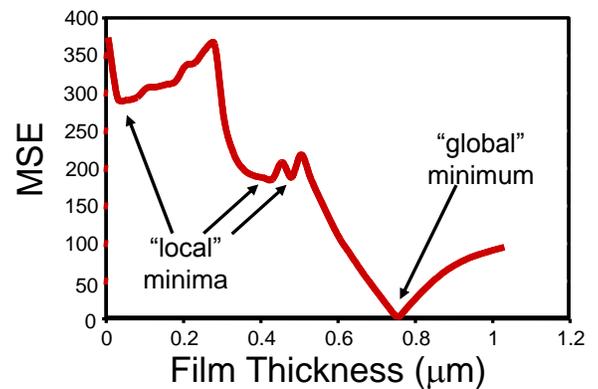
C-3
Silicon and SiO$_2$

Although the optical constants for most materials are variable, crystalline substrates can have very consistent properties. Silicon is one such material (at least in the ultraviolet to near infrared wavelength region). Thus, the silicon optical constants can be modeled using "known" values from the published literature. The values we choose were developed by Herzinger et al.[*]

This reference also provides excellent values for thermally grown SiO$_2$ films. There is a thin interface between the silicon substrate and the SiO$_2$ layer, which is also described in this reference.

*C. M. Herzinger, B. Johs, W. A. McGahan, J. A. Woollam, and W. Paulson, "Ellipsometric Determination of Optical Constants for Silicon and Thermally Grown Silicon Dioxide via a Multi-sample, Multi-wavelength, Multi-angle Investigation", *J. Appl. Phys.,* **83** (1998) 3323-3336.

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Effective Medium Approximation

The effective medium approximation (EMA) allows two or three materials to combine and form an "effective" mixed layer. Physical interpretation of EMA theory involves small particles of one material suspended within a host material. Under this approximation, the optical constants can be mixed to satisfy electromagnetic equations. In practice, the EMA is commonly used to describe surface or interfacial roughness, porous layers, and polycrystalline materials.

For further reading:

D.E. Aspnes, Thin Solid Films **89** (1982) 249.

H. G. Tompkins, *A User's Guide to Ellipsometry*, Boston: Academic Press, (1993) 246-251.

C-5
Surface or Interfacial Roughness

Surface roughness can be described using the Bruggeman effective medium approximation (EMA). This model mixes the optical constants of the surface material with void (air) in a 50:50 ratio. The approximation is valid when features are less than $1/10^{th}$ the wavelength of probe light. Larger roughness may scatter and depolarize light. Therefore, thick layers are not modeled correctly with an EMA. In practice, roughness is represented by a single, planar layer, with thickness varying to provide the best approximation of the surface properties.


Rough Surface · EMA approximation
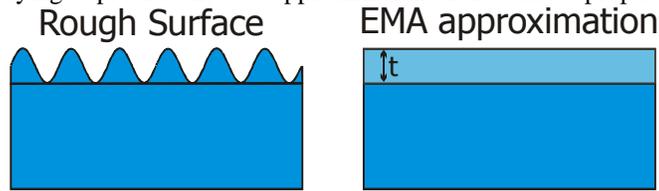
The EMA can also be used to mix two materials to approximate a rough interface. A 50:50 mixture of the material below and above the interface is assumed. This layer is used when the interfacial region is very thin – less than $1/10^{th}$ the wavelength of the probe light.

Rough Interface · EMA approximation
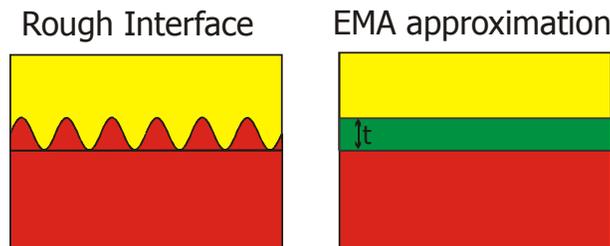
C-6
## Index Grading

If the index of refraction varies through a film (with depth), it may affect the ellipsometry measurement. Although it is difficult to describe the exact depth profile, the ellipsometer can estimate the "trend". Ellipsometry theory works with planar layers, so the index variation must be approximated as a series of "slabs" with varying index. The index at the surface can be larger or smaller than the index at the bottom of the film.

Index Variation · Graded Model · Depth Profile of Optical Constants at 1000nm
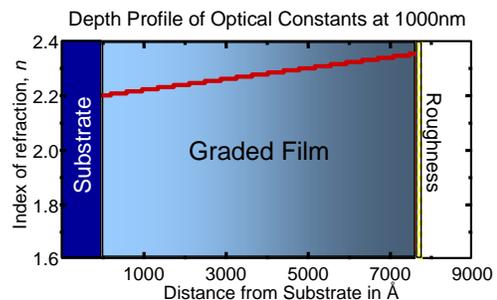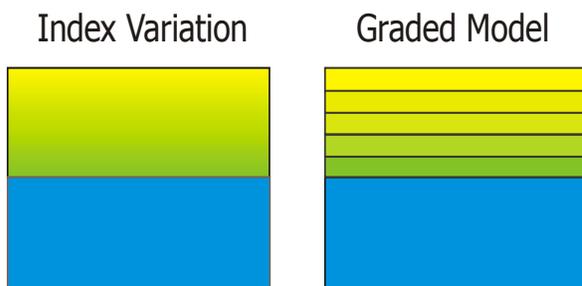
C-7 Thickness Nonuniformity

When a film varies within the measured spot, the ellipsometer measures an average thickness. Variation also "rounds" any sharp features in the experimental data. The effects caused by thickness non-uniformity are calculated using a series of slightly different thicknesses to correctly interpret the data. Non-uniformity can also introduce depolarization, so this can help quantify the thickness non-uniformity if the measurement includes depolarization (See Appendix B-6).

Sample with non-uniform film — Beam spot on sample
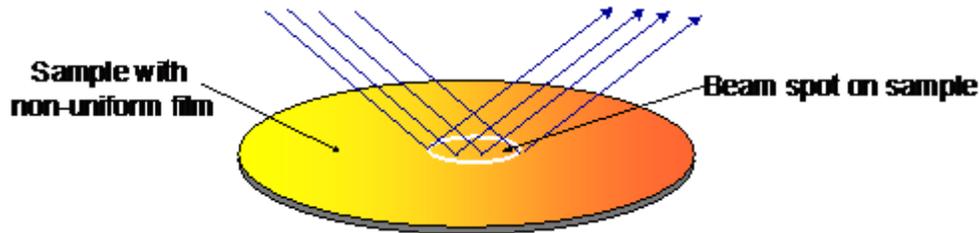
C-8 "Pseudo" Optical Constants

If a material is uniform, isotropic, optically thick (i.e., negligible reflection from the backside) with a smooth, abrupt surface; the optical constants can be directly calculated from the ellipsometry data, ρ, using:

$$\tilde{\varepsilon} = \tilde{n}^2 = \varepsilon_a \sin^2 \varphi \times \left(1 + \tan^2 \varphi \left(\frac{1-\rho}{1+\rho} \right)^2 \right)$$

where ε is the (complex) substrate dielectric function, ε_a is the ambient dielectric function, and φ is the angle of incidence of the light-beam. Of course we can still calculate these values even when the sample does not fulfill the stated criteria (e.g., the surface is rough, the substrate is not uniform or isotropic, there are one or more films on the substrate, or the substrate is not optically thick). In that case we replace ε (or ñ) with <ε> (or <ñ>), and describe them as pseudo-dielectric or pseudo-optical constants, respectively.

C-9 Wavelength-by-Wavelength Fit

Data analysis can often be extended into the absorbing region of a material by fixing the model (thicknesses determined from transparent region) and allowing the optical constants (*n* and *k*) to vary independently at each wavelength. This procedure offers the following advantages/disadvantages:

Advantage: Easy to use for many different materials, provided a transparent range is also measured to fix model thicknesses.

Advantage: Can measure complicated optical features (*n*, *k* that vary significantly with wavelength) that may be difficult to describe adequately with dispersion models.

Disadvantage: Does not maintain K-K consistency.

Disadvantage: Is susceptible to "branch-cuts", where data do not provide a unique answer. Difficult to detect whether answer is correct, unless KK consistency is investigated on resulting optical constants.

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C-10
Kramers-Kronig Relationship

The real and imaginary parts of the complex dielectric constant are not independent quantities – they are connected through the Kramers-Kronig relation. Absorption in the material also affects the index. Most oscillator models use KK consistency to maintain a physical relationship between the optical constants. A KK consistent dispersion model offers the following advantages/disadvantages:

Advantage: K-K consistent optical constants.

Advantage: Reduces the number of "free" parameters, such that thickness can be fit simultaneously with optical constants. This can clarify a model when transparent region is not sensitive to the actual sample structure.

Disadvantage: Difficult to setup for the first time and may vary from sample to sample.

Disadvantage: Can be difficult to accurately describe small features in the optical constants.

C-11
Dispersion Models (general)

The optical constants of a material vary with wavelength (dispersion). This dispersion can often be described with an equation. Dispersion models help reduce the number of parameters used to describe a material. Common dispersion models include the Cauchy and Sellmeier relationships for transparent materials and oscillator models (Lorentz, Drude, Gaussian, Tauc-Lorentz, Herzinger-Johs, …) for absorbing materials. Each of these dispersion relations is described in further detail in Appendix C-12 (transparent materials) and C-13 (absorbing materials).
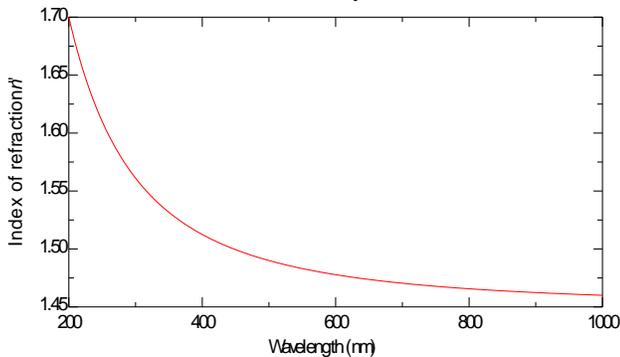
C-12
Transparent Models

Cauchy

The index of refraction, n(λ), for transparent materials can be described with the Cauchy dispersion model, given as:

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

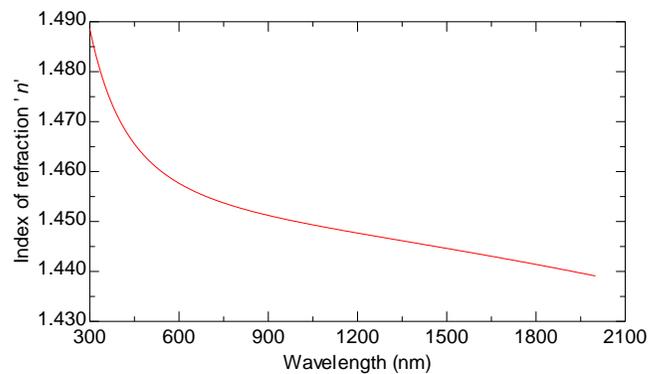where A_n, B_n, and C_n, are Cauchy parameters and λ is the wavelength in microns.


Cauchy

Sellmeier

The real part of the dielectric constant, $\varepsilon_1(\lambda)$, for transparent materials can be described using zero broadened oscillators outside the measured spectral range, based on Kramers-Kronig consistency (Appendix C-9). This dispersion model has the form:

$$\varepsilon_1 = Offset + \frac{A_a}{E_a{}^2 - E^2} + \frac{A_b}{E_b{}^2 - E^2} + ...$$

A variety of oscillator models are available; including Drude, Lorentz, Gaussian, Harmonic, Tauc-Lorentz, Herzinger-Johs™, and more. While each is different, they function in a similar manner. The $\varepsilon_2(\lambda)$ shape is described using oscillators with center energy, E_c, amplitude, A, and broadening, B. The $\varepsilon_1(\lambda)$ shape is linked to the $\varepsilon_2(\lambda)$ values through K-K consistency. There is also an ε_1 offset to account for absorption outside of the measured spectral range.
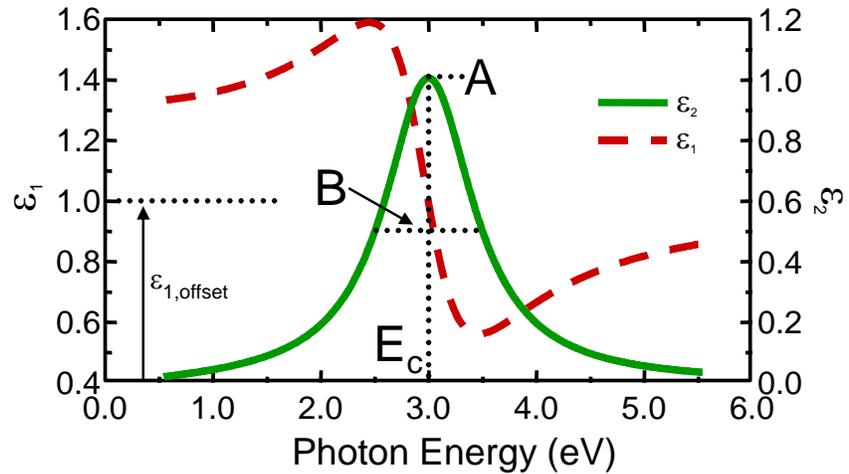
Lorentz

The Lorentz oscillator model is based on the assumption that electrons respond to a driving electric field (light beam) similar to a mass on a spring subject to a dissipative force. This classical representation of materials is often adequate for resonant absorptive processes. The dielectric response is given as:

$$\tilde{\varepsilon} = \frac{A}{E_0^{\ 2} - E^2 - i\gamma E}$$

where A is amplitude, E_0 is center energy, γ is broadening and E represents probe beam energy.

Tauc-Lorentz

The Tauc-Lorentz oscillator was developed by Jellison and Modine*. It is based on the Tauc joint density of states and the Lorentz oscillator with four parameters to describe ε_2: E_g, A, E_0 and C. The additional parameter (over 3-term oscillator models) is bandgap. Figure 16 compares a Tauc-Lorentz with a simple Lorentz oscillator. This model works particularly well for amorphous materials and will ensure that k=0 below the bandgap.

*G.E. Jellison, Jr. and F.A. Modine, "Parameterization of the optical functions of amorphous materials in the interband region," Appl. Phys. Lett. **69**, 371 (1996); Erratum, Appl. Phys. Lett. **69**, 2137 (1996).
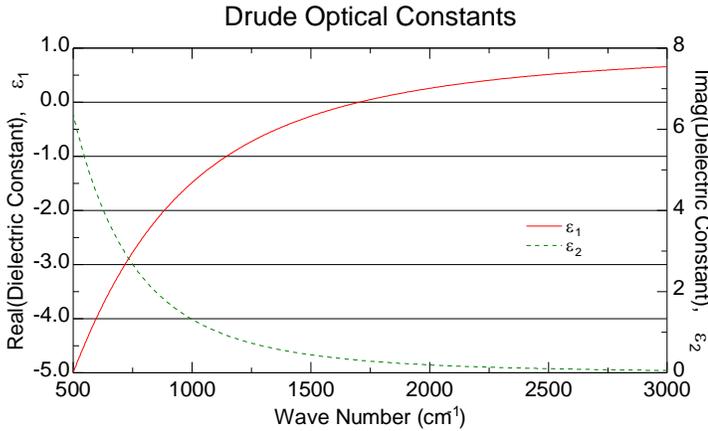
Optical Constants
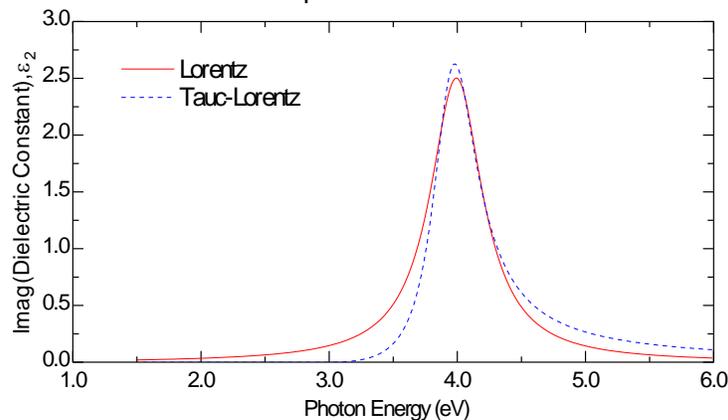
Drude

The Drude model is a Lorentz oscillator centered at zero energy, reducing to:

$$\tilde{\varepsilon} = -\frac{A}{E^2 + i\gamma E}$$

It is typically used to describe free carrier absorption present in metals, conductive oxides and heavily doped semiconductors.

Drude Optical Constants

Further Reading:
F. Wooten, *Optical Properties of Solids* (Academic Press, NY, 1972) p. 52.

A version of this model with resistivity and mean scattering time as free parameters is described by the following:

$$\varepsilon_{Drude}(E = \hbar\omega) = \frac{-\hbar^2}{\varepsilon_0 \rho(\tau \cdot E^2 + i\hbar E)} \quad \text{where} \quad \rho = \frac{m^*}{Nq^2\tau} = \frac{1}{q\mu N}$$

The adjustable Drude parameters are resistivity, ρ (Ω-cm) and scattering time, τ (sec). Other parameters of interest are m^* (carrier effective mass), N (carrier concentration - cm^{-3}), and μ (the carrier mobility in cm^{2}V^{-1}s^{-1}). The physical constants are $\hbar$ ({Plank's constant}/π), ε_o (the vacuum dielectric constant), single electron charge q (1.6x10^{-19} C).

An IR-specific parametric model for silicon consists of a Drude model for free-carrier effects superimposed on a Sellmeier model. The Sellmeier accounts for absorption at high energies outside this measurement range. The Sellmeier is adjusted to match previously published optical constants for silicon extrapolated from UV-Vis-NIR ellipsometric measurements*.

Further Reading:
T.E. Tiwald, D.W. Thompson, J.A. Woollam, W. Paulson, R. Hance, *Thin Solid Films* **313-314** 661 (1998).
P. Y. Yu and M. Cardona, *Fundamentals of Semiconductors*,3rd Ed. (Springer-Verlag, Berlin, 2001) pp. 306-310.
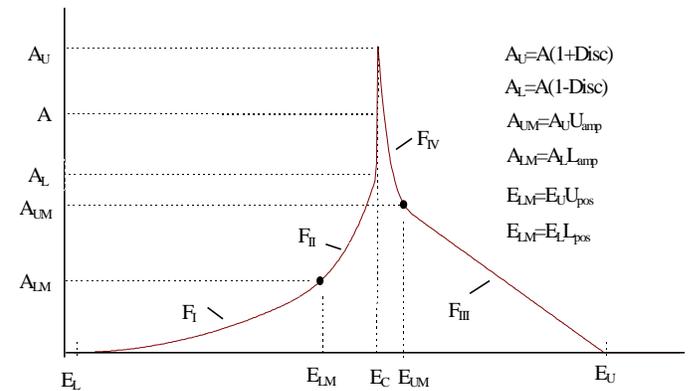J. Humlíček, *Thin Solid Films* **313-314**, 656 (1998).
*Silicon UV-NIR optical constants from C.M. Herzinger, B. Johs, W.A. McGahan, J.A. Woollam and W. Paulson, *J. Appl. Phys.* **83**, 3323 (1998).

Gaussian

The Gaussian oscillator features a Gaussian line shape for the ε_2 spectra, with a KK consistent line shape for the ε_1 spectra:

$$\varepsilon_{n2} = A_n e^{-\left(\frac{E - E_n}{Br_n}\right)} + A_n e^{-\left(\frac{E + E_n}{Br_n}\right)}$$

$$\varepsilon_{n1} = \frac{2}{\pi} P \int_{R_g}^{\infty} \frac{\xi \varepsilon_{n2}(\xi)}{\xi^2 - E^2} d\xi$$

Herzinger-Johs

A more advanced oscillator model is the patented Herzinger-Johs™ parametric model*. This model features up to 12 parameters to describe each oscillator. Its sophistication and flexibility make it the best choice for a wide range of materials.
*Patent #5,796,983, Herzinger et. al., "Dielectric Function Parametric Model, and Method of Use".

The B-Spline layer describes the optical constant dispersion using a series of control points which are equally spaced in photon energy (eV)[1]. The appropriate spacing is controlled depending on the sample and optical features to be described.

The B-Spline layer uses b-spline (also known as basis-spline) curves to represent the dielectric function (ε_1 and ε_2) versus photon energy. Basis spline curves are smooth and continuous in the 0th, 1st, and 2nd derivatives. B-spline curves have many desirable properties for modeling dielectric functions:

- b-spline curves and their derivatives (up to the spline order minus one) are continuous.
- since the basis functions depend only on the node positions, the node amplitudes which define the resulting curve are linearly independent, which greatly increases computation efficiency
- the Kramers-Kronig (K-K) integral can be applied to the b-spline recursion formula to generate K-K consistent basis functions (i.e., the $\varepsilon 1$ curve is defined by the K-K transform of $\varepsilon 2$)
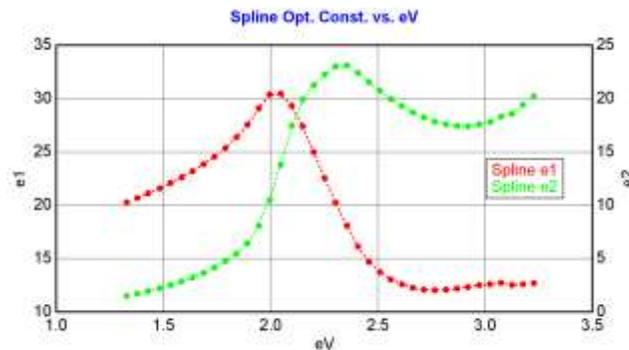
After a series of compositions has been measured, the resulting optical constants can be stored in a single model to describe the ALLOY. This allows the optical constants to be accessed for any composition, with advanced interpolation (critical point shifting algorithm*) for measured values between the original series composition. The resulting composition is relative to the original composition entered to create the alloy model.

*P. G. Snyder *et al*, J. Appl. Phys., **68** 5925 (1990)

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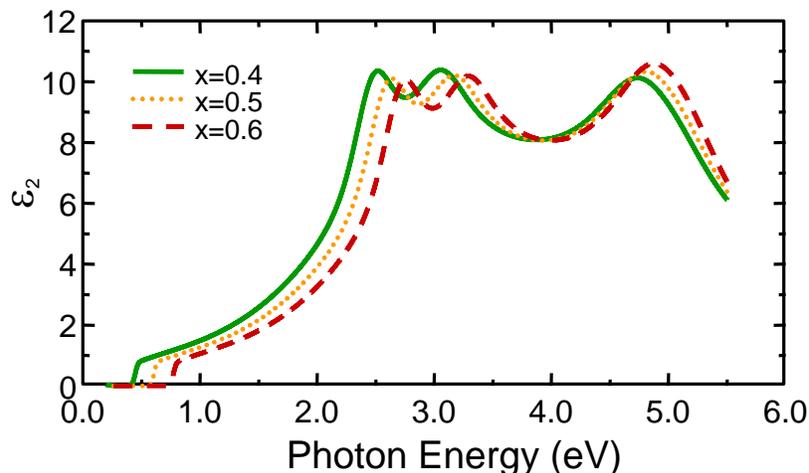
[1] B. Johs and J.S. Hale, "Dielectric function representation by B-splines", Phys. Stat. Sol. (a) 1-5 (2008).

J.A. Woollam Co., Inc.
Ellipsometry Solutions

A very potent means of eliminating strong parameter correlations from complex models is the technique of multiple sample analysis. Any time two or more samples are known to have some physical property in common, the analysis of both (or all) samples may be performed simultaneously, with the common physical property coupled across the models for the different samples

The reason why we wish to fit more than one sample at a time is that we can force parameters in the optical model for the various samples to be identical for more than one sample, thereby hopefully eliminating correlations which prevent the unique determination of the desired model for a single sample alone.

For example, we cannot usually uniquely obtain the thickness and optical constants of thin metal films on opaque substrates, but we can usually obtain a unique solution for the two thicknesses and one set of optical constants of two thin films of the same metal on opaque substrates. Suppose we measured two samples consisting of thin aluminum films on silicon wafers. The aluminum films are nominally identical but of differing thickness. Multiple sample analysis allows us to fit data from both samples simultaneously, varying the aluminum film thickness on each sample and a single set of aluminum optical constants, forced to be identical for both films.

For further reading:

B. Johs, J. A. Woollam, C. M. Herziner, J. Hilfiker, R. Synowicki, and C. L. Bungay, "Overview of Variable Angle Spectroscopic Ellipsometry (VASE), Part II: Advanced Applications", *SPIE Proc*. **CR72** (2000) 29.