

Copyright 1999 Society of Photo-Optical Instrumentation Engineers.

This paper was published in *Critical Reviews of Optical Science and Technology Volume CR72* (proceedings of a conference held 18-19 July 1999 in Denver, Colorado, ©1999 by SPIE, Bellingham, WA) and is made available as an electronic reprint with permission of SPIE. Single print or electronic copies for personal use only are allowed. Systematic or multiple reproduction, or distribution to multiple locations through an electronic listserver or other electronic means, or duplication of any material in this paper for a fee or for commercial purposes is prohibited. By choosing to view or print this document, you agree to all the provisions of the copyright law protecting it.

REPRINT

Critical Reviews of
Optical Science
and Technology



Volume CR72

Optical Metrology

Ghanim A. Al-Jumaily

Seagate Technology

Editor

Proceedings of a conference held

18–19 July 1999

Denver, Colorado

Overview of Variable Angle Spectroscopic Ellipsometer (VASE), Part I: Basic Theory and Typical Applications

John A. Woollam*, Blaine Johs, Craig M. Herzinger,
James Hilfiker, Ron Synowicki, and Corey L. Bungay

J.A. Woollam Co., Inc.,
645 'M' St. #102, Lincoln, NE 68508

©1999 by the Society of Photo-Optical Instrumentation Engineers
Box 10, Bellingham, Washington 98227 USA. Telephone 360/676-3290.

Overview of Variable Angle Spectroscopic Ellipsometry (VASE), Part I: Basic Theory and Typical Applications

John A. Woollam*, Blaine Johs, Craig M. Herzinger, James Hilfiker,
Ron Synowicki, and Corey L. Bungay

J.A. Woollam Co., Inc., 645 'M' St. #102, Lincoln, NE 68508

ABSTRACT

Variable angle spectroscopic ellipsometry (VASE) is important for metrology in several industries, and is a powerful technique for research on new materials and processes. Sophisticated instrumentation and software for VASE data acquisition and analysis is available for the most demanding research applications, while simple to use software enables the use of VASE for routine measurements as well. This article gives a basic introduction to the theory of ellipsometry, references "classic" papers, and shows typical VASE applications. In the following companion paper, more advanced applications are discussed.

Keywords: Ellipsometry, optical properties, spectroscopy, metrology

1. VASE THEORY

1.1. Introduction

The mathematical theory for ellipsometric analysis is based on the Fresnel reflection or transmission equations for polarized light encountering boundaries in planar multi-layered materials^{1,2}. These come from solutions to Maxwell's equations³. The ellipsometric measurement is normally expressed in terms of Psi (Ψ) and Delta (Δ):

$$\tan(\Psi) \cdot e^{i\Delta} = \rho = \frac{r_p}{r_s} \quad (1)$$

where r_p and r_s are the complex Fresnel reflection coefficients of the sample for p- (in the plane of incidence) and s- (perpendicular to the plane of incidence) polarized light, illustrated in Figure 1. Spectroscopic Ellipsometry (SE) measures the complex ratio ρ as a function of wavelength⁴⁻¹¹. Variable Angle Spectroscopic Ellipsometry (VASE) performs the above measurement as a function of both wavelength and angle of incidence¹².

* Correspondence: Email: jwoollam@jwoollam.com; WWW: www.jwoollam.com;
Telephone: 402-477-7501; FAX: 402-477-8214

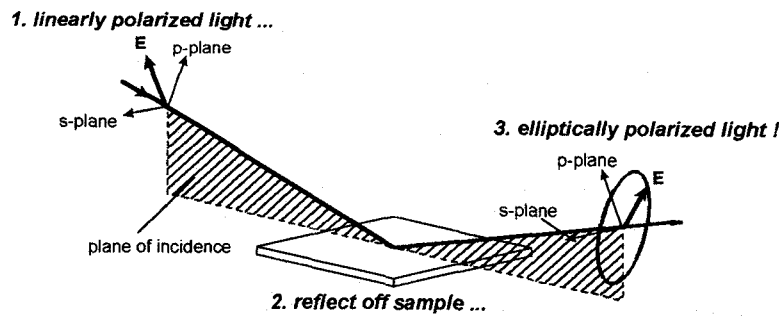
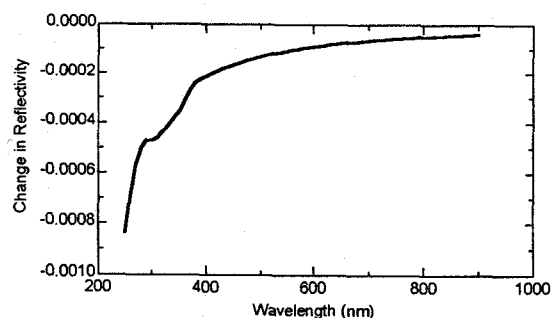


Figure 1. Interaction of polarized light with a sample.

Because ellipsometry measures the *ratio* of two values it is highly accurate and reproducible, and no reference material is necessary. Because it measures a phase quantity ' Δ ' (as well as an amplitude ratio), it is very sensitive even to the presence of very thin films. Use of Spectroscopic Ellipsometry (SE) results in increased sensitivity to multiple film parameters, and as well, eliminates the 'period' problem, associated with interference oscillations in thick films. Another feature of SE is that it measures data at the wavelength of interest, which is of particular importance for industrial problems such as development of lithography at new wavelengths. Adding multiple angles to spectroscopic capability (VASE) provides new information because of the different optical path lengths traversed, and it optimizes sensitivity to the unknown parameters.

To illustrate the thin film sensitivity advantage of ellipsometry over traditional reflectivity measurements, consider the following figures. Figure 2 shows the calculated change in reflectance caused by a thickness change of 0.1nm on a 10nm thick SiO_2 layer on crystalline Silicon. A typical reflectometer system can not accurately measure intensity values to better than 0.1%, and therefore a reflectivity measurement is not very sensitive to small changes in ultra thin film thicknesses. (Reflectance *precision* may be better than 0.1%, but data *accuracy* is needed for thickness accuracy.) The ellipsometric sensitivity to a similar change in thin film thickness is shown in Figure 3. As typical ellipsometers can accurately measure Ψ and Δ to better than 0.02° and 0.1° respectively, it is clear that film thickness changes down to the sub-Å scale can easily be resolved with this technique.

Figure 2. Calculated change in reflectivity for a 0.1nm thickness change on a 10nm SiO_2 on Silicon sample.

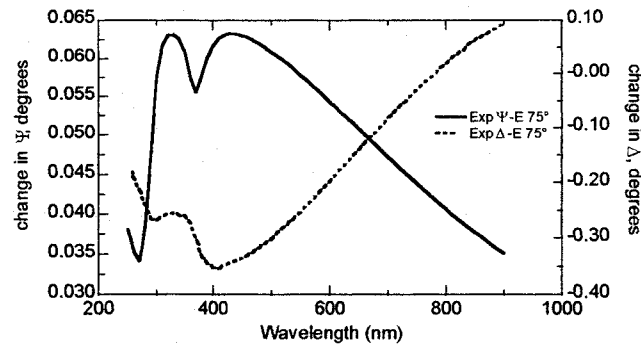


Figure 3. Calculated change in ellipsometric parameters Ψ and Δ for a 0.1 nm thickness change on a 10 nm SiO_2 on Silicon sample.

1.2. What Can Be Determined by VASE?

Many desired material parameters can be extracted by VASE analysis, including layer thickness, surface and/or interfacial roughness, and optical constants. The ellipsometric Ψ and Δ data measured on a bulk sample can be directly inverted into the 'pseudo-optical' constants of the material, assuming that surface oxide and/or roughness effects are negligible (this transform is given by Equation 2, in which ' ϕ ' is the angle of incidence, and ' ρ ' is the complex ellipsometric ratio defined in Equation 1). In addition, VASE is also sensitive to gradients in material properties vs. depth in the film, optical anisotropy, and any physical parameter that depends on the material optical constants (such as crystallinity, alloy composition, and temperature). A full optical and microstructure analysis of real materials, including multi-layered structures, requires use of regression analysis, as will be explained in a following section.

$$\langle \epsilon \rangle = \langle \epsilon_1 \rangle + i \langle \epsilon_2 \rangle = \langle \tilde{n} \rangle^2 = \langle (n) + i(k) \rangle^2 = \sin(\phi)^2 \cdot \left[1 + \tan(\phi)^2 \cdot \left(\frac{1 - \rho}{1 + \rho} \right)^2 \right] \quad (2)$$

1.3. Instrumentation Basics

Figure 4 shows the block diagram layout of a rotating analyzer spectroscopic ellipsometer (RAE). Light from an arc lamp passes through a monochromator, and a narrow spectral band of collimated light then passes through a polarizer, reflects at oblique angle off the sample under study, passes through a second, rotating polarizer (analyzer) and enters a detector. The angle of incidence in this ellipsometer is computer controlled, and is generally in the range of 50° to 80° , depending on sample. Other ellipsometer configurations (shown in Figure 5) are the Rotating Polarizer (RPE), Rotating Compensator (RCE), and Polarization Modulation (PME). The predominant configuration in the early history of ellipsometry was the Null Ellipsometer. In recent years, however, the rotating element, or modulation-based ellipsometers have become more popular¹³.

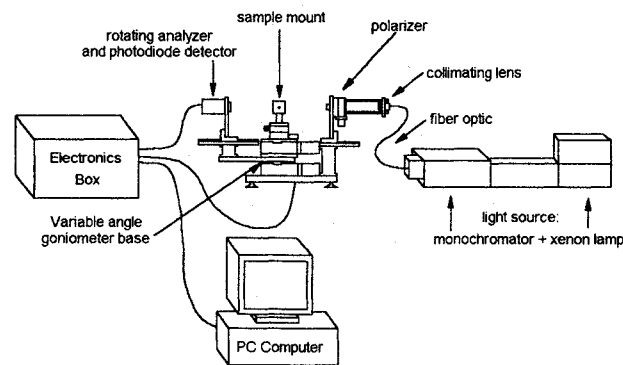


Figure 4. Block diagram of a rotating analyzer spectroscopic ellipsometer.

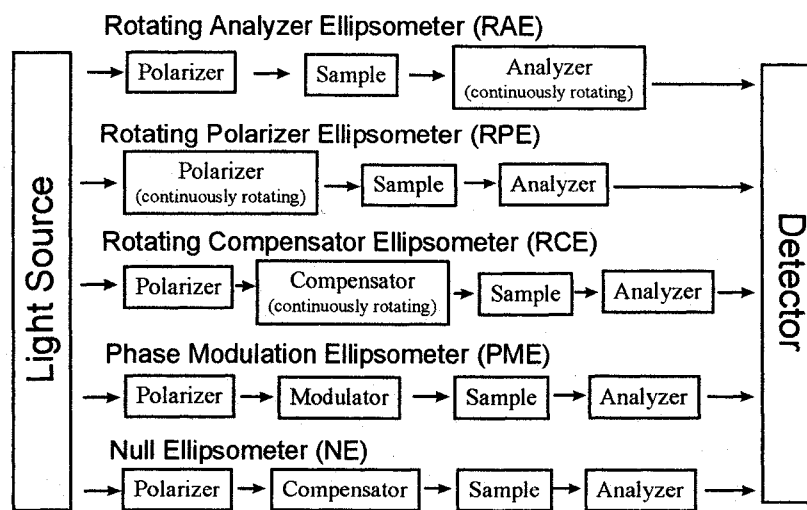


Figure 5. Block diagram of various ellipsometer configurations.

Each ellipsometer configuration has different features and merits. With null ellipsometers, the azimuth of each optical element is rotated to extinguish beam intensity at the detector. Traditionally null ellipsometry data acquisition is slow, involving manual adjustments. Also, it is difficult to make spectroscopic measurements, thus for years laser sources were used. One positive attribute is that null ellipsometers are accurate, and there are low systematic errors.

Polarization Modulation Ellipsometers can operate at very high modulation rates, $\sim 50\text{kHz}$, and thus have the potential for very rapid data acquisition provided the probe beam is intense enough (e.g. a laser) to achieve a reasonable signal-to-noise figure. In a scanning wavelength spectroscopic configuration acquisition rates are usually limited by the comparative low signal strength of a broad-band source and by monochromator slewing speed. Because the typical PME modulator is not inherently spectroscopic (e.g. drive voltage adjusted for each wavelength) and the modulation rate is typically very high, PME type systems are not well suited to simultaneous measurements at multiple wavelengths using an array based detector. Overall, spectroscopic PME

systems are difficult to construct and calibrate, require very stable modulators are required for high accuracy, and are noisy when Ψ is near 0° or 45° (depending the particular instrument configuration).

Rotating Polarizer or Rotating Analyzer Ellipsometers (RPE or RAE) can be highly accurate and are easy to construct. However, they are less sensitive to Δ when Δ is near 0° or 180° , and secondly, the acquisition speed is theoretically limited by the rotating element (15-50Hz is typical). However, source intensity typically limits acquisition speed to about 1 second per measurement. The RPE configuration places a static (typically adjustable) polarizer after the sample. It is therefore immune to polarization sensitivity effects in the detector, however, the RPE system is sensitive to residual polarization in the source beam. Because monochromators tend to produce partially polarized light, in the RPE configuration, the monochromator almost always comes after the sample and “white light” (full spectrum of source) illuminates the sample, which sometimes results in solarization of the optical elements and the measurement beam can modify photosensitive samples. Conversely, the RAE system, with its static polarizer before the sample, is not affected by residual source polarization but may require calibration of detector polarization sensitivity for highest accuracy. In the RAE system, the monochromator is almost always before the input polarizer and only one wavelength at a time propagates through the system

The Rotating Compensator Ellipsometer (RCE) configuration has advantages over the previous configurations in that it uses two static polarizers which eliminate sensitivity to both residual source polarization and detector polarization sensitivity. Furthermore, the RCE measures Ψ and Δ over their full ranges with almost equal accuracy. The primary hurdle to RCE systems is designing the compensating element to be close enough to ideal over an acceptable spectral range. The maximum speed is similar to RPE and RAE style systems, but the RCE configuration is compatible with array based detectors for truly parallel spectroscopic measurement. The RCE configuration is discussed in more detail in the companion paper.

Other optical configurations have been used, but those described above are the main ones used today. Specifications of major instrument types can be obtained from manufacturer's product literature or from published research papers of instruments developed in universities. This is not the place to give details of all the possibilities, however much ellipsometry is now done spectroscopically, sometimes at a fixed angle of incidence, but often at variable angles, with manual or automated control of angle of incidence. The commercially available spectral range covers 150 nm to 33 μm , and somewhat wider ranges have been used in academic research. Also, spectroscopy is done using monochromators, diode or CCD arrays, or Fourier transform methods. The other general configuration choice is between *in situ* (on a process chamber) and *ex situ* (on table-top). Some instruments can perform intensity transmittance and reflectance measurements, as well as reflection or transmission ellipsometry. Both horizontal and vertical sample orientations are available. For complex anisotropic materials, automated sample rotation stages have been used. Cryostat sample chambers have also been adapted to allow VASE measurements as a function of temperature, typically from 4K to well above room temperature.

1.4. Data Analysis Theory

Ellipsometry does not directly measure film thicknesses or optical constants, it measures Ψ and Δ . To extract useful information about a sample, it is necessary to perform a model dependent analysis of the ellipsometric Ψ and Δ data. Figure 6 outlines this process.

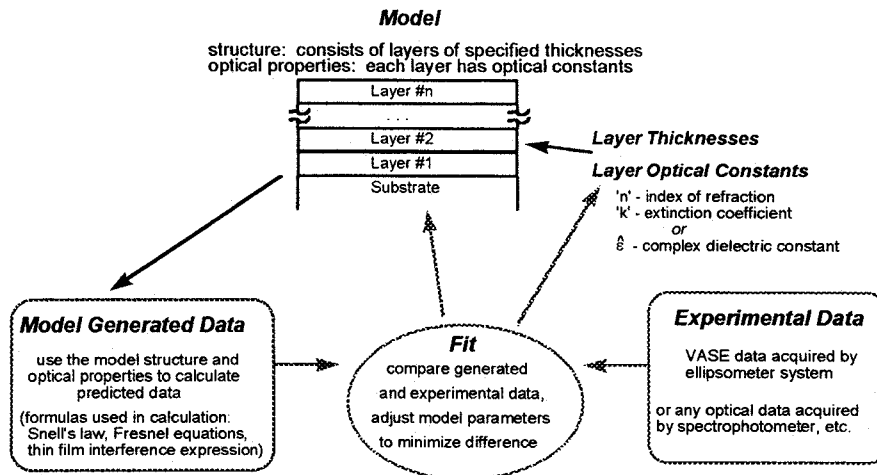


Figure 6. Flowchart of VASE Data analysis procedure.

First, data are acquired covering the desired spectral range and angles of incidence. A model for the optical structure of the sample is then constructed. For example, this may include a substrate and a single film on top, or substrate plus film with roughness on top, or more complex multilayer structures. In the example section below, we will show the analysis of quite complex materials systems.

Second, the Fresnel equations along with the assumed model are used to predict the expected Ψ and Δ data for the wavelength and angles of incidence chosen. Figure 7 shows light propagating from the ambient media into a simple system where the material is a bulk solid, or has a single film on a substrate¹. Analytic algebraic expressions can be written for predicting Ψ and Δ as functions of optical constants and layer thickness. Optical constants ('n' and 'k') describe how light propagates through a given material. The algebra of calculating Ψ and Δ will not be presented here, but can be found in standard references.¹

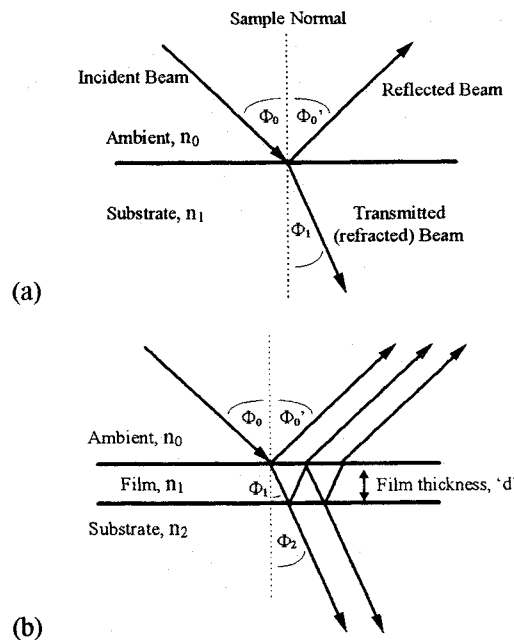


Figure 7. (a) Reflection of light at material interfaces, and (b) multiple reflections within a film, which result in thin film interference effects.

In the case of more complex materials systems, the algebra becomes tedious, and analytical expressions are not usually derived. Rather a matrix multiplication procedure is followed in which each layer and boundary of the structure is represented by a matrix, and a computer is used to do the matrix multiplication, yielding predicted ellipsometric data for a multilayer structure.

The third part of the process described in Figure 6 is to compare the actual measured Ψ and Δ with the predictions of the model based on Fresnel equations, assuming values of the optical constants and thicknesses. While the forward calculation, simulating measurements from a specific model, is straightforward, the inverse problem of determining what the sample parameters were that produced the actual experimental results is a more difficult problem. An obvious, but often tricky, feature of all model-based data analysis procedures is in picking the model to use and deciding what parameters to try and determine from the analysis. The analysis procedure is usually called data fitting because the adjustable model parameters are varied to find the best fit of the generated data to the actual experimental data. The most common fit parameters are thicknesses and optical constants. In some cases, good optical constants are available in published tables. In other cases ellipsometric analysis can be used to determine both optical constants and thicknesses, as well as other parameters of the system.

Various fitting algorithms have been tried, but by far the most commonly used is the Marquardt-Levenberg algorithm. Again, this will not be described here, as it is quite involved, and is well documented elsewhere¹⁴. The object is to quickly determine the model which exhibits the minimum difference (BEST FIT) between the measured and

calculated Ψ and Δ values. The (Root) Mean Squared Error (MSE) is used to quantify the difference between the experimental and predicted data. A smaller MSE implies a better model fit to the data. The MSE can be normalized by the standard deviations on the experimental data, so noisy points are weighted less heavily. The MSE function commonly used¹⁵ is given by Equation 3. Minimizing the MSE (or Fitting the Data) by iterative non-linear regression is illustrated in Figure 10, which shows that convergence for a system with one, or just a few variables is quite rapid.

$$MSE = \sqrt{\frac{1}{2N - M} \sum_{i=1}^N \left[\left(\frac{\Psi_i^{Mod} - \Psi_i^{Exp}}{\sigma_{\Psi,i}^{Exp}} \right)^2 + \left(\frac{\Delta_i^{Mod} - \Delta_i^{Exp}}{\sigma_{\Delta,i}^{Exp}} \right)^2 \right]} \quad (3)$$

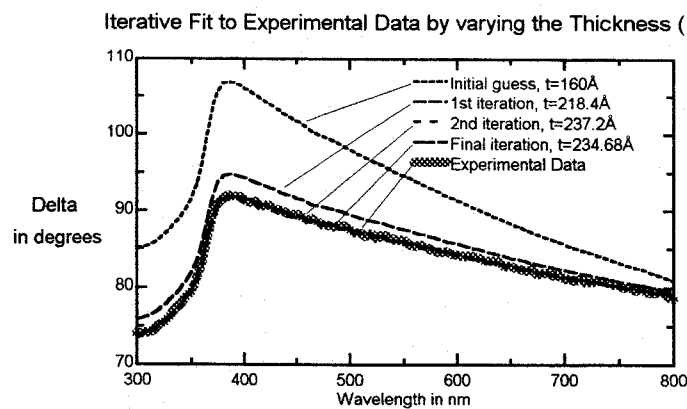


Figure 8. The Levenberg-Marquardt non-linear regression algorithm converges very quickly for most analyses.

Such regression analysis requires the correct model to achieve good fits to the experimental SE data. If the model does not adequately represent the true sample structure, then good agreement between experiment and theory (such as seen in Figure 8) is not found, and the model needs to be reformulated. For most materials and structures good optical models can be found, and the process works marvelously. Typically, the simplest model is first assumed, and then successively more complex models are tried until an excellent data fit is achieved. The model must be complex enough to adequately model all of the structure in the data. As well, there should also be enough information content in the data to uniquely determine all model parameters. That is, the danger in making the model more complex is that parameters become correlated, in which case multiple sets of parameters will give the same good MSE fit. Parameter correlation (and how to reduce it) will be discussed in detail in a subsequent section of the paper. Also in a later section we illustrate a few of the many cases in which ellipsometric analysis works extremely well. *All* examples in this article are from *real* experimental VASE data.

1.5. Classic Example of VASE Analysis: SiO₂ on Si

A classic sample which is often characterized by ellipsometry consists of an SiO₂ film on a Si substrate. In the example below, the SiO₂ film thickness and index of refraction is extracted from the analysis of VASE data. To model the mild dispersion in index of refraction, a Cauchy formula (Equation 4) is used to calculate the SiO₂ refractive index as a function of wavelength. The model fit parameters for this analysis were the thickness of the SiO₂ film, and the 3 Cauchy parameters A, B, and C. After 5 iterations, the regression algorithm converged to the near perfect data fits shown in Figure 9, and final parameter values of: Thickness=3537Å, A=1.44, B=4.22×10⁻³, C=1.89×10⁻⁵ (the fit MSE = 2.25). The resulting SiO₂ optical constants are also shown in Figure 10.

$$n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4}, \quad k(\lambda) = 0 \quad (4)$$

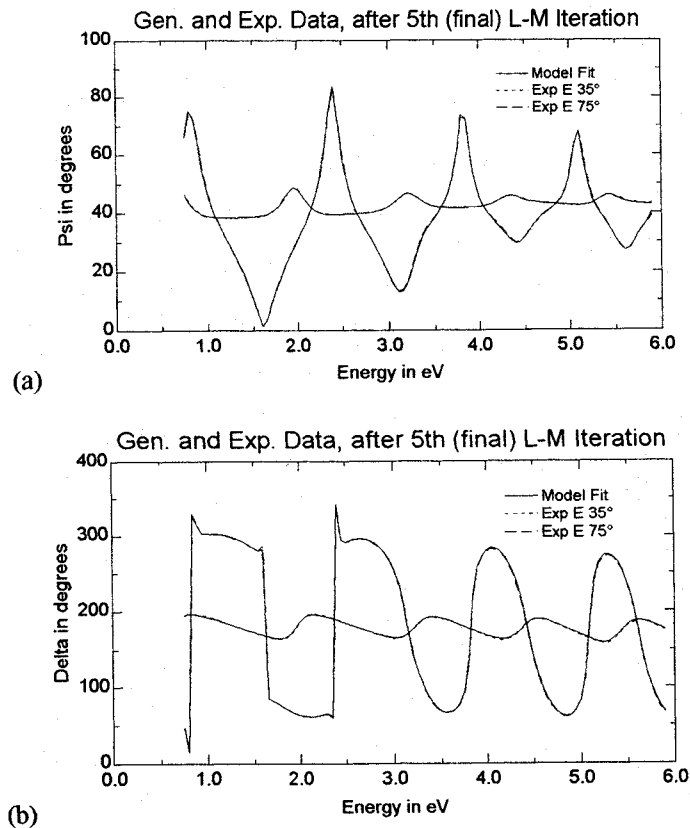


Figure 9. Experimental and Model Fit VASE data from a SiO₂ on Silicon sample. Note the near perfect data fits; on this scale the solid Model Fit curves lie directly on top of the dashed Experimental curves.

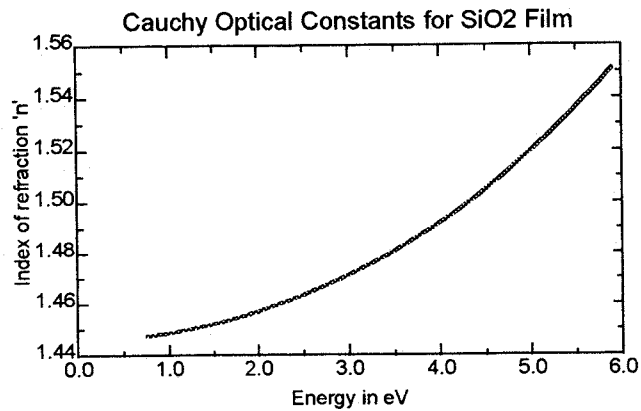


Figure 10. SiO₂ optical constants determined from the VASE data analysis, parameterized by the Cauchy dispersion formula.

2. IMPORTANT CONSIDERATIONS FOR VASE ANALYSIS

2.1 Initial Guesses for Parameter Values

Figure 11 illustrates an important consideration in analyzing VASE data: if the initial guess for a parameter value (thickness in the present case) is too far from the actual value, the regression algorithm can land on a secondary minimum in the MSE, thus yielding an erroneous value for the parameter. In Figure 11, there are at least three MSE minima shown, but only the 'global minimum' gives the correct thickness. To ensure that the true 'global' minimum MSE is found, the regression algorithm can be started with a wide range of initial parameter values (some commercial software does this 'global searching' automatically). Fit convergence to the same final parameter values with different initial values is also a good test of the 'uniqueness' of the fit (the related problem of parameter correlation is discussed later).

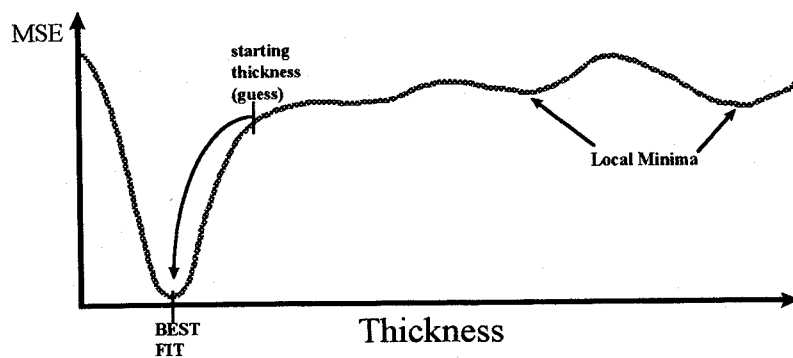


Figure 11. Illustration of Secondary MSE Minima.

2.2. Building an Appropriate Optical Model

To extract accurate material properties from VASE analysis, it is very important to build an appropriate optical model which has enough flexibility to accurately fit the experimental data. As an example, consider the VASE data shown in Fig. 12 which was acquired on a bulk $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ sample. The goal of the VASE analysis was to accurately determine the alloy fraction 'x', which was nominally 0.21 for this sample (a composition-parameterized optical constant database was used for determine the alloy fraction, the details of which are not important here). The resulting fit parameters from the first analysis (shown in Figure 12) in which an ideal bulk optical model (i.e. no surface overlayer) was used are: $\text{MSE}=48.9$ and $x=0.147$. As the MSE value was unacceptably high, and the fit was noticeably poor, another more complex optical model was tried. In this second model, a surface roughness layer was added to the bulk $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ substrate. Surface roughness is optically modeled by a layer with optical constants derived from a 50-50% mixture of air (void) and the substrate optical constants (using the Bruggeman effective medium approximation). The fit results for this model are shown in Figure 13, and the resulting fit parameters were: $\text{MSE}=3.92$, $x=.222$, and surface roughness thickness= $18.9\text{\AA}$. By adding a single fit parameter to the analysis (surface roughness), the MSE was reduced by an order of magnitude, and the resulting alloy fraction was in much better agreement with the nominal value. In this example, the more complicated 'surface roughness' optical model is easily justified, and in fact, the surface roughness model *must* be used to obtain reliable results in the parameter of interest (alloy composition in this case). As a sidenote, VASE-determined roughness values have also been corroborated by other techniques such as AFM²⁰.

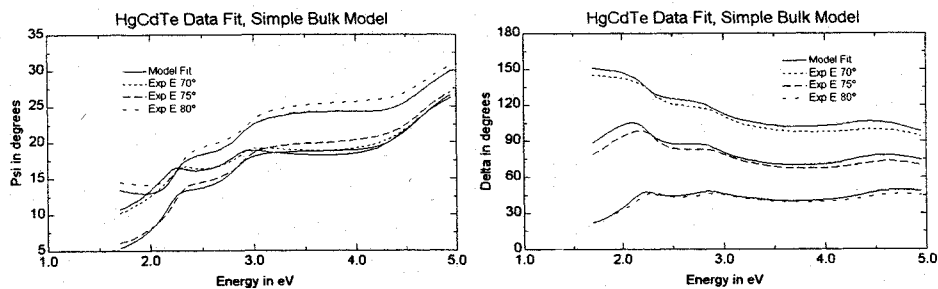


Figure 12. VASE data fits for a $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ sample, analyzed by a simple bulk model; note the poor agreement between the solid Model Fit curves and the dashed Experimental curves.

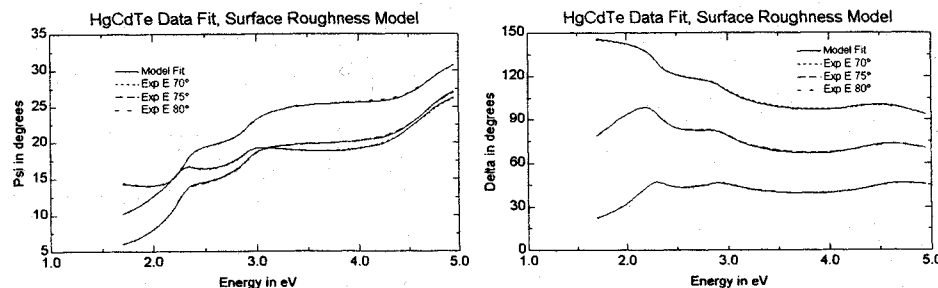


Figure 13. Excellent VASE data fits on a bulk $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ sample with surface roughness included in the optical model.

2.3. Parameter Sensitivity and Correlation

Parameter sensitivity is simply a measure of how much the experimental data would be expected to change for a given change in the parameter. It is obvious to note that having parameter sensitivity greater than the accuracy level of the measurement is a necessary prerequisite to determining that parameter from a data fit, and that the *potential* accuracy with which the parameter can be determined increases with increasing sensitivity. However, that potential accuracy will be reduced or eliminated if correlation with other parameter(s) exists.

Parameter correlation is a condition of the data fitting process which arises if the sensitivity of two or more parameters singly, or in combination, exhibit the same spectral signature. It is not limited to ellipsometric analysis, but is a general feature of any model-dependent fitting process. What this means is that even if a good fit is obtained with sensitivity to all fit parameters, not all the parameters will necessarily have been uniquely determined. Correlation is important to understand, and is often not sufficiently considered because it does not affect the ability to fit the experimental data, but it does place a limit on the information available from an ellipsometric data analysis. Two-parameter correlation information is a natural output of most fitting algorithms.¹⁴

One technique to deal with correlation is to simplify the model to reduce unnecessary fit parameters. The previous section demonstrated that the optical model needs to be sufficiently complex to fit the data. There are however a limitless set of sample models with increasing complexity which would also fit the data, so some limits on complexity are needed. Generally, the simplest model which fits the data is probably best. Simplest meaning, for example, that existing optical constants are preferred over fitting new ones, that interface roughness should be ignored unless necessary, and so forth. Each additional level of complexity needs to produce an improved fit, or the complexity can not be proved necessary. (Of course, a more complex model can never truly be excluded as the correct physical model.) Sometimes including an additional physical constraint such as rigorously enforcing the Kramers-Kronig relation for a set of optical constants can break the correlation. Additional data, including non-ellipsometric data (multi-data-type analysis, as in the following example) and data from different samples (multi-sample analysis), might be added to the fitting process to change the spectral sensitivity signatures for the parameters, thus breaking the correlation. (The follow-on companion paper discusses some of these advanced techniques in more detail.) In other cases, it may be possible to redefine the fit parameters in the model to make the parameters more orthogonal. For example, it may be more informative to make an index difference between films ($\Delta n = n_2 - n_1$) and the average index ($n_{ave} = \frac{1}{2}(n_2 + n_1)$) the fit parameters instead of n_2 and n_1 directly. Also, consider whether the parameters which are correlated are really of primary interest, and if not, then it is reasonable to ignore the correlation. The mere existence of correlation among the fitting parameters does not invalidate the procedure, it just limits the amount of unique information that can be properly extracted.

The following example demonstrates a case of parameter correlation when VASE data alone is available and then shows how the addition of intensity transmittance data breaks the correlation. Consider the analysis of VASE data acquired from a silver film

on glass sample, in which it is desired to simultaneously determine the silver layer thickness and optical constants. The problem is that identical data fits over a range of silver film thicknesses from 330 – 430 Å can be obtained. Depending on the assumed thickness, the silver optical constants 'n' and 'k' shift to compensate while yielding the same good fit. That is, the silver film thickness and optical constants are correlated parameters, and neither correct thicknesses nor correct optical constants can be determined from VASE data alone. (See Fig. 14)

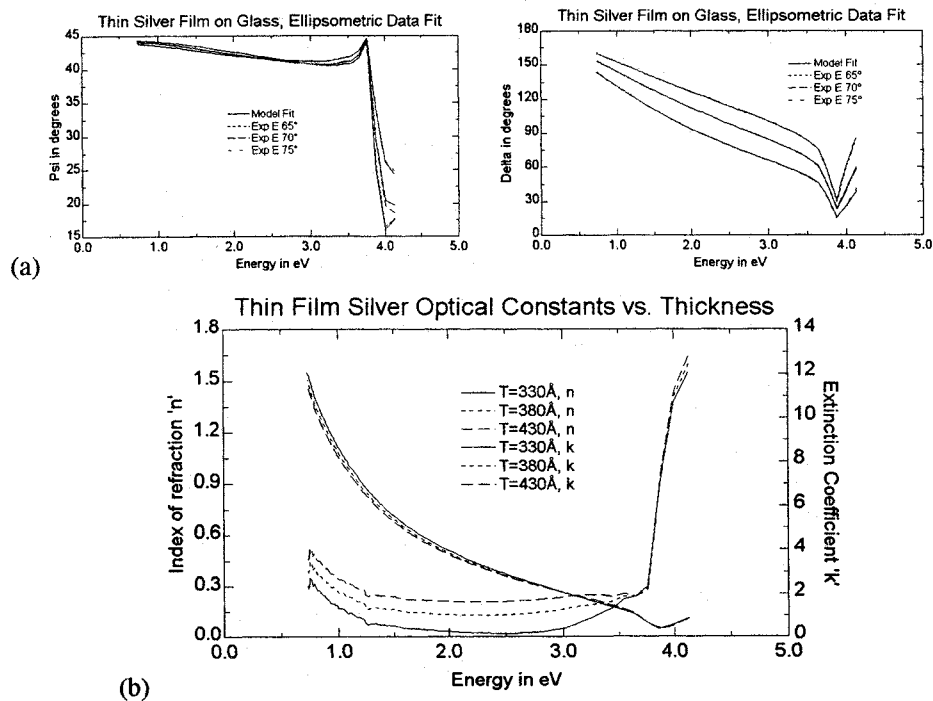


Figure 14. (a) Equivalent VASE data fits obtained over a range of assumed thickness for a silver film on glass sample. (b) Optical constants for the silver film, extracted over a range of layer thicknesses.

To de-correlate the silver film thickness and optical constants, spectroscopic transmission data from the sample was combined with the VASE data, and regressed simultaneously¹⁷. Only a single, unique silver thickness can fit both the ellipsometric and transmission data, as shown by Figure 15. As a result of the combined VASE and transmission analysis, the silver film thickness was determined to be 341.7 Å with a 7.4 Å surface roughness layer, and unique silver optical constants were simultaneously extracted. Addition of transmission data not only de-correlated the model parameters, it also provided enough extra information to determine surface roughness, that is, it enabled the use of a more complex optical model.

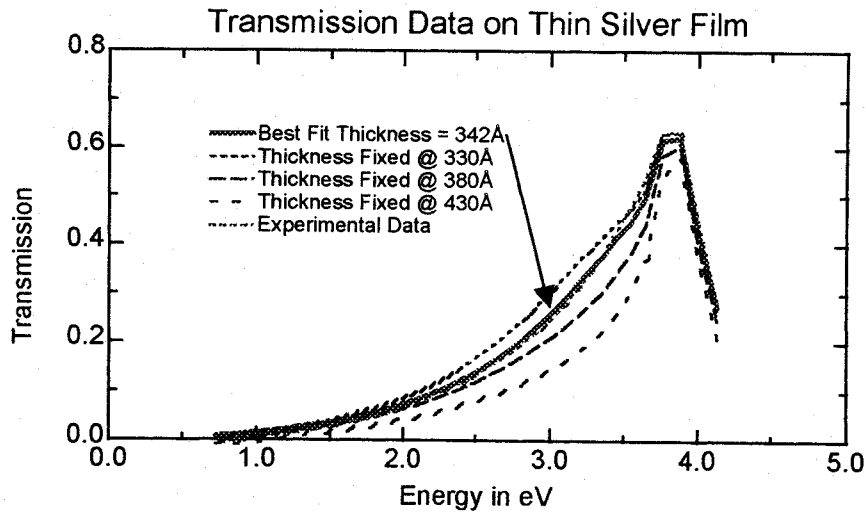


Figure 15. Experimental and model generated transmission data for thin silver film on glass sample, illustrating the unique determination of film thickness.

2.4. Maximizing Sensitivity: Optimum Angle of Incidence

Figure 16 shows the sensitivity in the ellipsometric Δ parameter to a 0.1 nm change in a thin oxide thickness. Note that the maximum sensitivity to the measurement of thickness is just above and just below 75° angle of incidence for wavelengths greater than about 600 nm. (At shorter wavelengths, the high sensitivity moves to slightly higher angles of incidence.) High sensitivity occurs near the Brewster angle¹, which is defined in Figure 17; this generally corresponds to $\Delta \approx 90^\circ$ for samples with very thin, or no, overlayers.

Thus an important part of making VASE measurements is to identify the angles and wavelengths at which the data is most sensitive to the parameters of interest. This can be done by simulations, such as that shown in Figure 16. In general, the regions of sensitivity can be highly parameter-dependent, for example, some parameters may have high sensitivity at 65°, while others may be more sensitive to data at 75° (and likewise for various wavelength ranges). To achieve acceptable sensitivity to multiple parameters, Variable Angle Spectroscopic Ellipsometric (VASE) measurements, performed at an appropriately chosen range of angles, are often required.

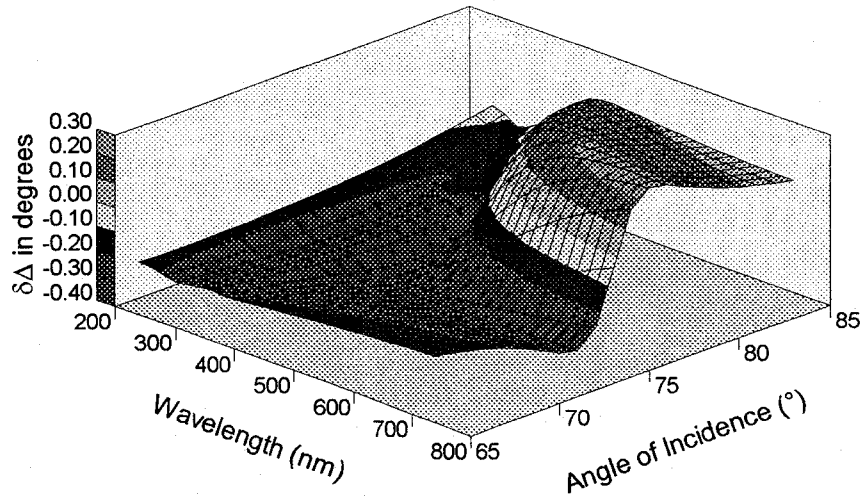


Figure 16. Sensitivity in the ellipsometric Δ parameter to a 0.1 nm change in SiO_2 layer thickness vs. Wavelength and Angle of Incidence.

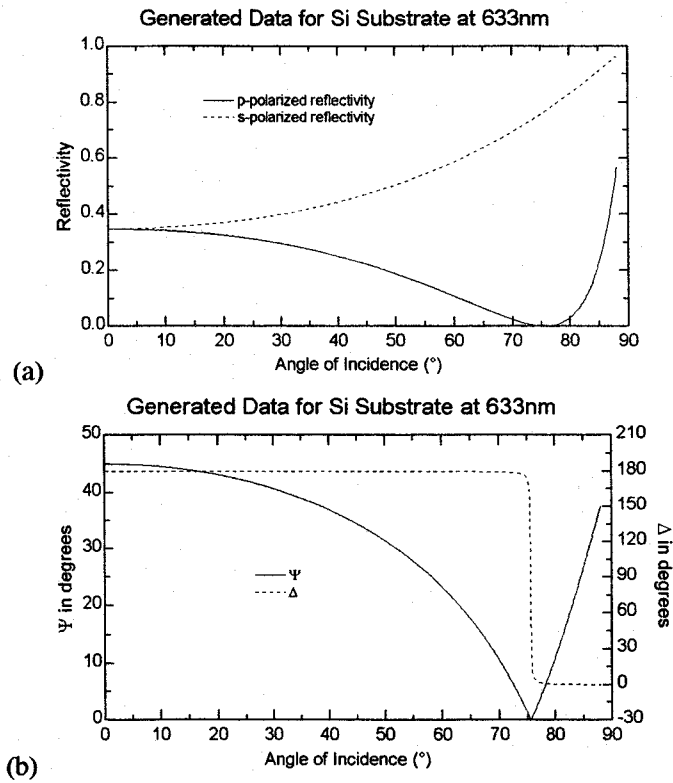


Figure 17. Model generated (a) reflectivity and (b) ellipsometric data vs. angle of incidence for a Silicon substrate at 633 nm. The Brewster angle is defined as the angle where the p-polarized reflectivity and Ψ are minimized and $\Delta \approx 90^\circ$, which is near 76° in this case.

3. TYPICAL VASE EXAMPLES FOR INDUSTRIAL APPLICATIONS

3.1 Semiconductor Industry

3.1.1. ONOPO / Si Stacks

A common material system in the Si-based semiconductor industry with important metrology needs consists of a thin-film stack of oxide on nitride on oxide on poly-silicon on oxide on crystalline silicon: ONOPO / Si. A VASE measurement can determine all 5 layer thicknesses, as well as the poly-Si optical constants. Example VASE data and analysis are given in Figure 18. Notice that VASE data are acquired and fit at four angles of incidence. The optical constants of poly-Silicon depend strongly on crystallinity, which in turn depends on process conditions (Figure 19).

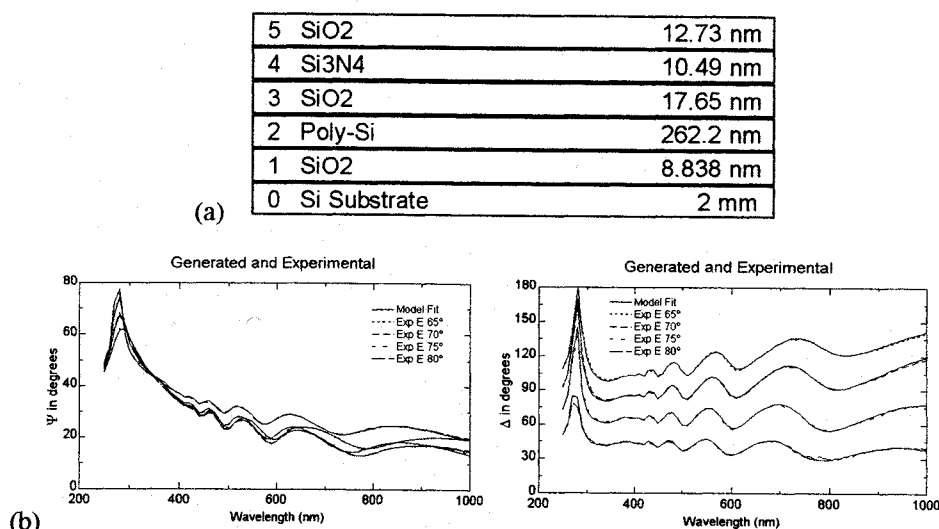


Figure 18. Optical model (a) and VASE data fits (b) from a ONOPO/Si stack.

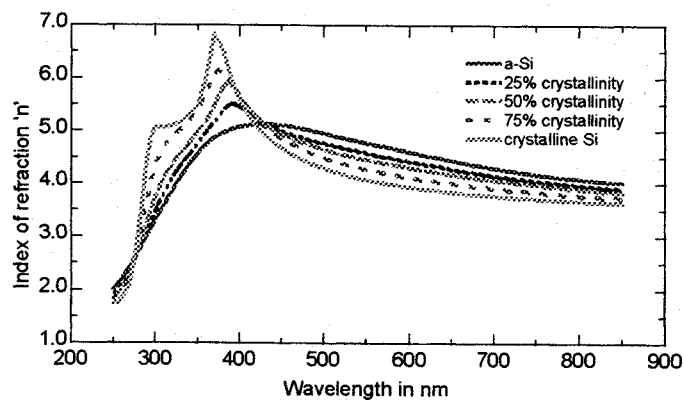


Figure 19. Index of Refraction of Poly-Si as a Function of Crystallinity.

3.1.2. Optical Constants of Photoresist

Ellipsometers are used regularly in the optical characterization new photoresists, and for process control of photoresists on the production line. In Figure 20, the optical constants for a typical photoresist are shown²³, both before and after 'bleaching' (i.e., 'exposing' the resist by UV light), which induces large changes in the optical properties of the resist. To prevent exposure of the photoresist by the measurement beam, it was extremely important to have the monochromator placed before the sample in the VASE system. Another photoresist example (Figure 21) involves a multilayer of photoresist with an antireflective coating (ARC) beneath it. Both layer thicknesses can be extracted from the VASE data, but only by including UV data in the analysis, as this spectral region exhibits optical contrast between two materials.

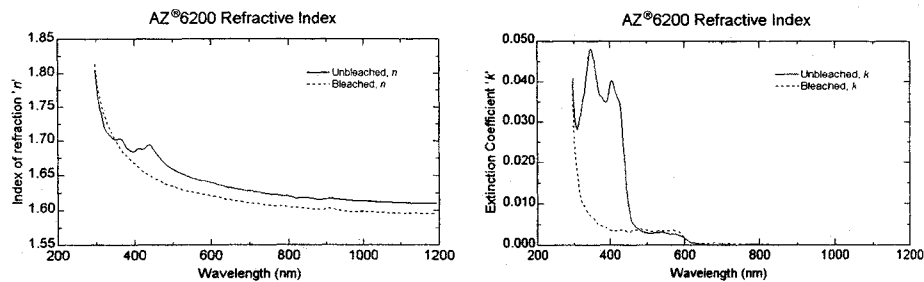


Figure 20. Optical constants of photoresist determined by VASE measurements, before and after bleaching (by exposure to UV light).

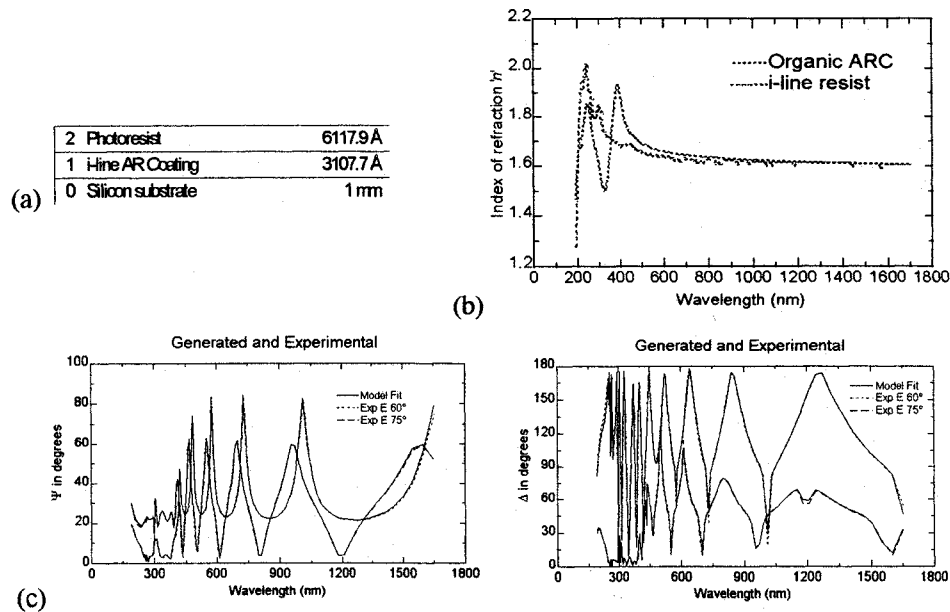


Figure 21. Multilayer photoresist on anti-reflective coating (ARC) example: (a) optical model, (b) optical properties of the resist and ARC films (note the optical contrast in the UV spectral range), and (c) VASE data fits.

3.1.3 Compound Semiconductors: $\text{Al}_x\text{Ga}_{1-x}\text{As}$ Multilayer Structure

The thicknesses and compositions of complex compound semiconductor structures can also be determined by VASE measurements. Figure 22 shows an example in which VASE unambiguously determined the surface oxide thickness, three layer compositions, and eight layer thicknesses. Note that some of the layer thicknesses and compositions were coupled together (via the definition of 2 and 3 period superlattices in the optical model) in the analysis to reduce parameter correlation. Due to the in-run reproducibility of the deposition technique used to fabricate the sample (MBE in this case), this assumption is readily justified. Ellipsometric data at multiple angles (three in this case) helped to extract the many thicknesses and alloy ratios with high precision and accuracy. The uniqueness of the fit was demonstrated by the convergence of the regression analysis to the same final values over a wide range of initial parameter guesses.

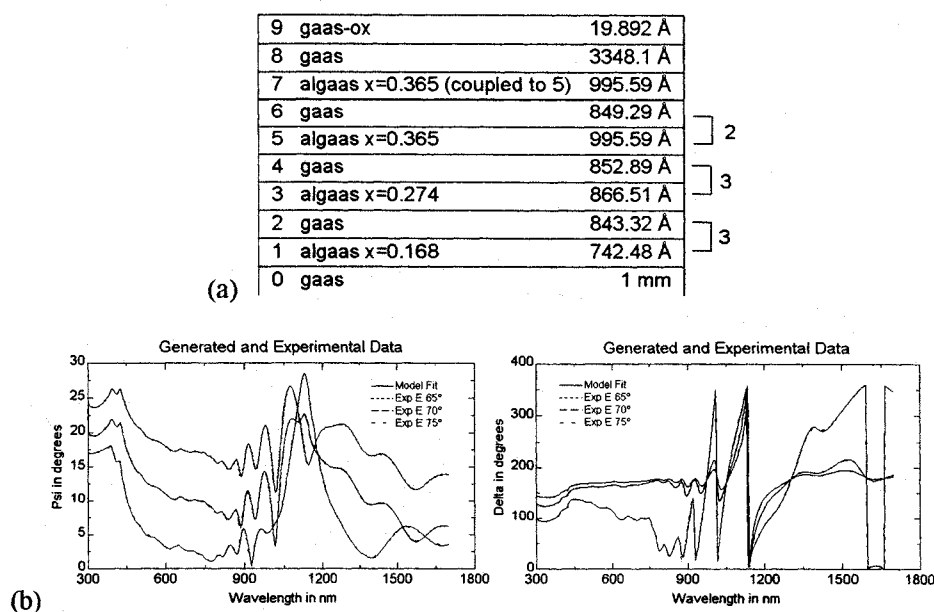


Figure 22. VASE analysis of a $\text{Al}_x\text{Ga}_{1-x}\text{As}$ multilayer structure: (a) optical model, and (b) data fits. Note the near perfect fits to *all* of the structure in the data, which were essential to simultaneously and accurately extract all the layer thicknesses and compositions.

3.2. Optical Coatings Industry

3.2.1. Five Layer Hi-Lo Index Stack

In this example (Figure 23), 5 layer thicknesses and 3 sets of optical constants in a 'Hi-Lo' index multilayer stack were simultaneously determined. To achieve this result, multiple data types were included in the analysis: VASE data acquired from front side and back side of the sample (both of which included the reflections from the opposite side of the transparent substrate), and spectroscopic transmission acquired at normal incidence. The Cauchy dispersion formula was used to model the dispersion in index of refraction for the three materials in the stack. From a simultaneous analysis of all the data, unambiguous results for this multilayer structure were obtained: five layer thicknesses (plus a surface roughness thickness), and the indices of refraction for three materials.

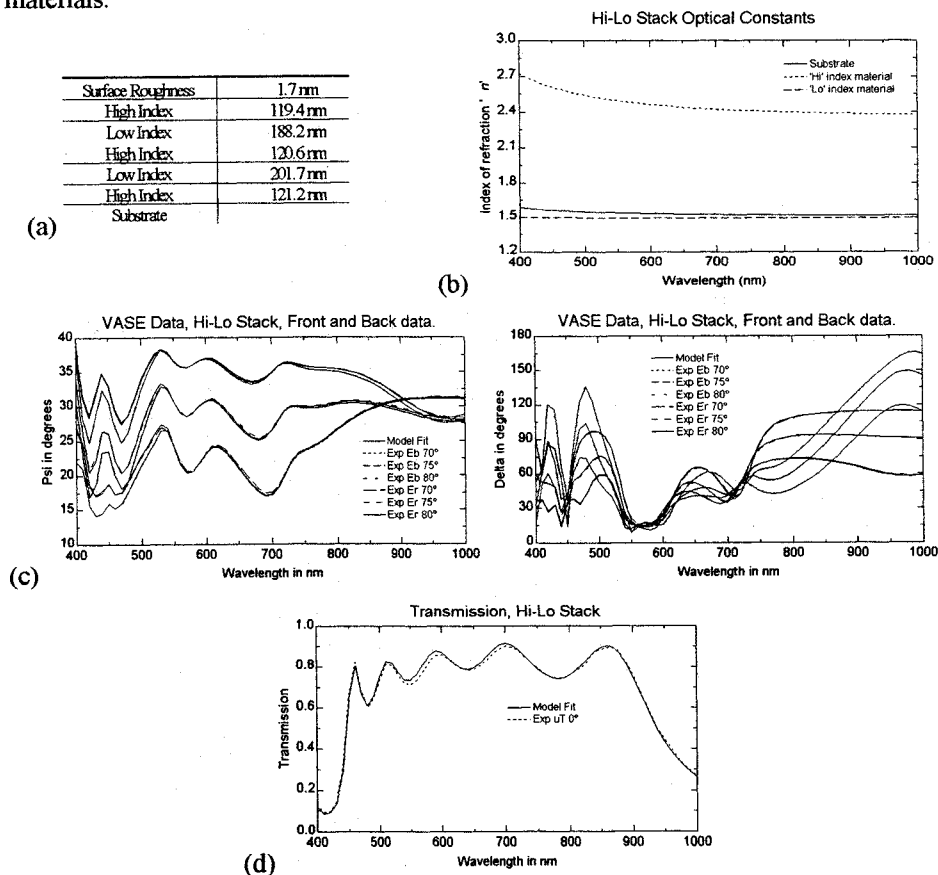


Figure 23. Analysis of a 5 layer Hi-Lo index optical stack using multiple data types: (a) best fit optical model, (b) extracted indices of refraction for the three constituent materials in the stack, (c) ellipsometric data fits, in which the 'Eb' curves correspond to ellipsometric data acquired on the front side of the sample (including the 'backside' reflection), and the 'Er' curves correspond to ellipsometric data acquired in the 'reverse' direction, i.e. from the backside of the sample (including the 'frontside' reflection), and (d) fit to normal incidence transmission data.

3.2.2. Variations in Optical Coating Index vs. Depth

In this example, the initial requirement was to simply determine the film thickness and index of refraction for a Si_3N_4 coating on glass. However, the first modeling attempt of the VASE data (shown in Figure 24a) was not successful, as evidenced by the poor data fits and high MSE value. A second model, which included a surface roughness layer, was also tried (Figure 24b), but this optical model did not adequately fit the experimental VASE data either. After extensive trial and error, an optical model was found which provided excellent fits to the data (Figure 24c). This best fit model had an optically less dense 'interfacial' layer embedded in the film, the optical properties of which were modeled by a 50% Bruggeman EMA mixture of the Si_3N_4 film index and void (similar to the optical modeling of surface roughness). After the VASE analysis of this sample, it was learned that the film was deposited in two passes, thus explaining the double layer with embedded interface solution. This example conclusively demonstrates the sensitivity of VASE measurements to non-uniformity (gradients) in film optical properties as a function of depth in the film.

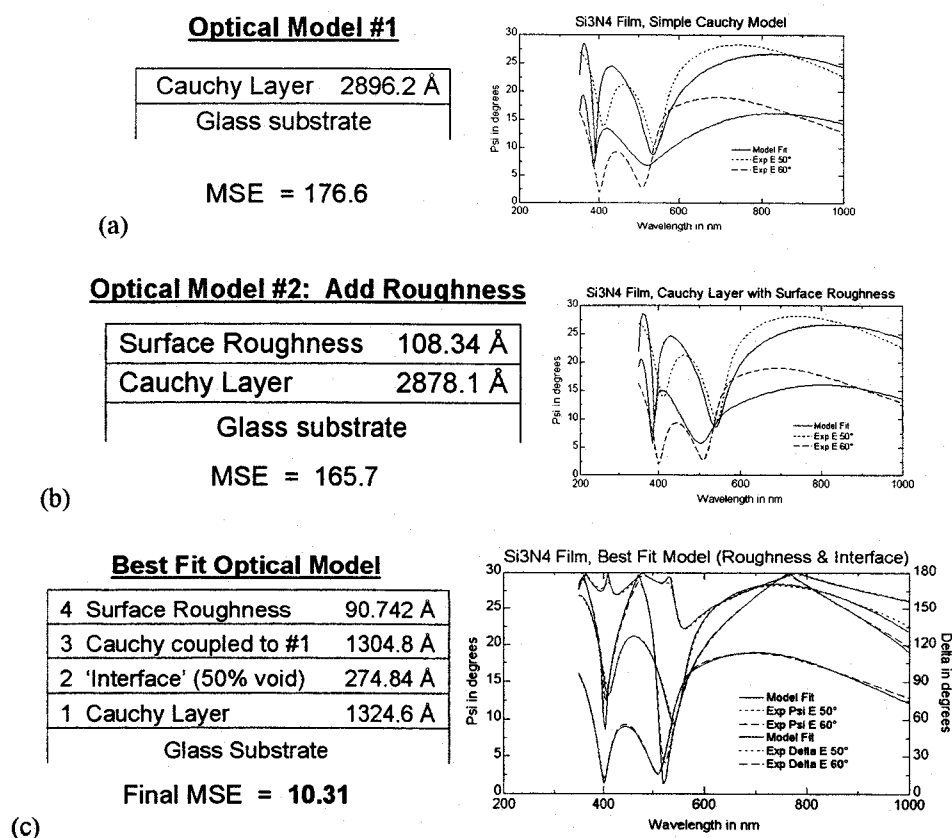


Figure 24. Progression of optical models used to analyze a Si_3N_4 coating on glass sample: (a) simple single film model, (b) single film with surface roughness, and (c) best fit optical model, which included a less dense 'interfacial' layer within the film (this was introduced by the two-pass deposition of the film).

3.3. Data Storage Industry

3.3.1. Diamond-Like Carbon (DLC)

Due to their excellent protective and lubricative properties, diamond-like carbon (DLC) films are commonly applied to hard disk media and read-write heads. DLC films are usually made by plasma CVD using a mixture of hydrocarbon gasses, such that a wide range of film mechanical properties can be obtained by adjusting the process conditions. As there is a correlation between variations in the DLC mechanical and optical properties (see Figure 25), VASE is very useful in the monitoring of DLC processes. The sensitivity of VASE to ultra-thin films is also advantageous when characterizing DLC coatings, which are typically $<100\text{\AA}$ (Figure 26).

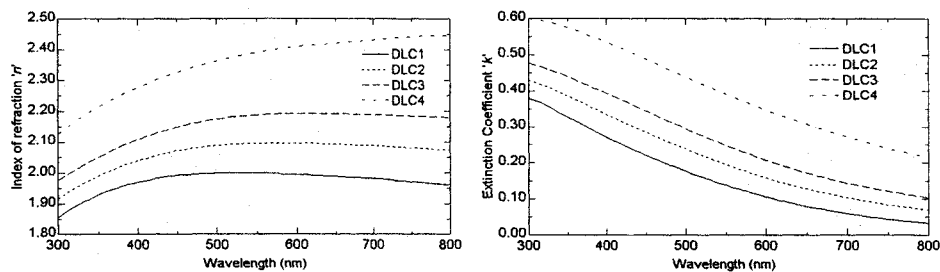


Figure 25. Variation in diamond-like carbon (DLC) optical constants; these optical constants were extracted from a VASE analysis of four different samples, in which the DLC deposition conditions were systematically varied.

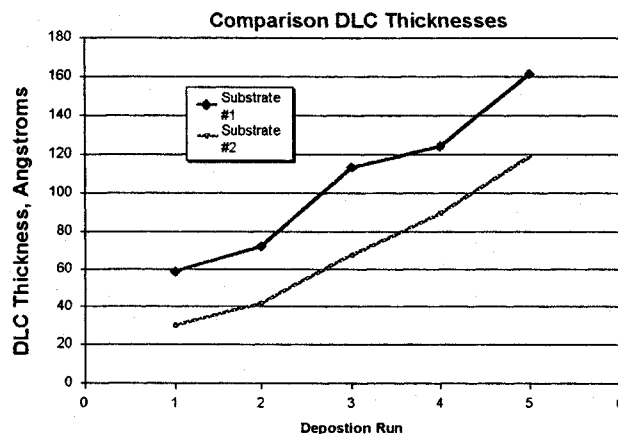


Figure 26. Systematic study of DLC films coated on two different substrates; the high sensitivity of VASE to ultra-thin films enable precise thickness determination in this application.

3.3.2. Thickness of Thin Magnetic Films

The performance of advanced read heads is critically dependent on the thickness of thin magnetic films. Accurate characterization of such films requires accurate thin film optical constants for the metallic layers of interest, which may differ significantly from the bulk optical constants found in the literature. By performing VASE analysis on a thin magnetic layer deposited on a thick dielectric film, it is possible to simultaneously and accurately extract optical constants of the metallic layer, along with the metal and dielectric film thicknesses. In this analysis, the multiple angles of ellipsometric data provide a change in the optical path length through the layers (this effect is enhanced by the thick underlying dielectric film²¹), which breaks the correlation between the thickness and optical constants of the metal film. See Figure 27.

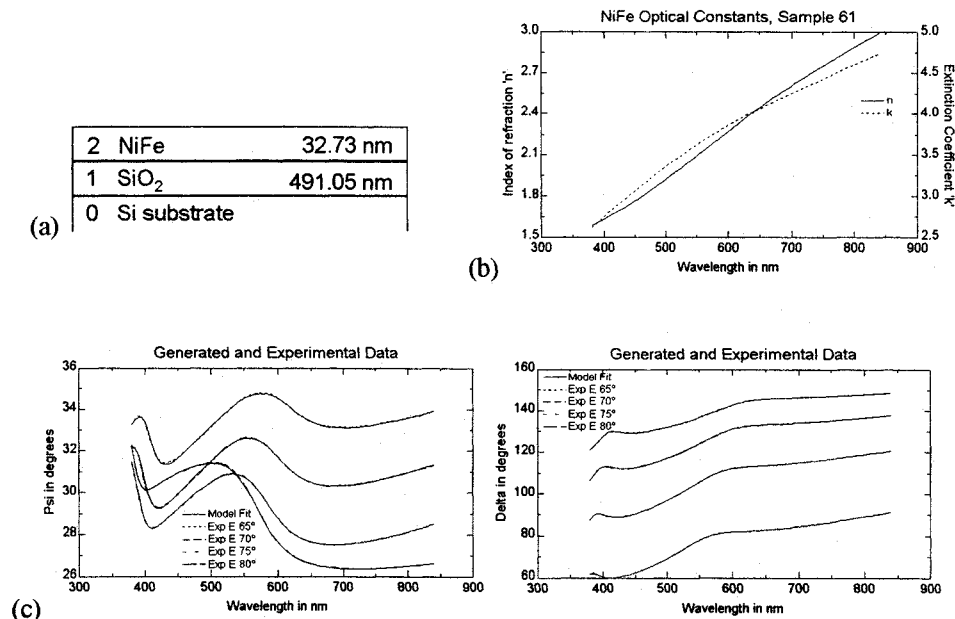


Figure 27. Simultaneous thickness and optical constant determination for a thin NiFe layer deposited on a thick SiO₂ film on Si: (a) optical model, (b) resulting NiFe optical constants, and (c) VASE data fits.

3.4. Flat Panel Display Industry

3.4.1. Indium Tin Oxide (ITO) Films

Indium Tin Oxide (ITO) is a transparent electrically conducting film used extensively in the flat panel display industry as a large-area electrode. Optical characterization of ITO films is challenging, as the ITO optical properties are highly dependent on the film deposition and annealing process. Furthermore, significant gradients in the optical constants (vs. depth in the film) are commonly observed in ITO films. A VASE analysis of a typical ITO sample²² is presented and described in Figure 28. To adequately fit the experimental VASE data and properly characterize the ITO film, a complex graded optical model is required.

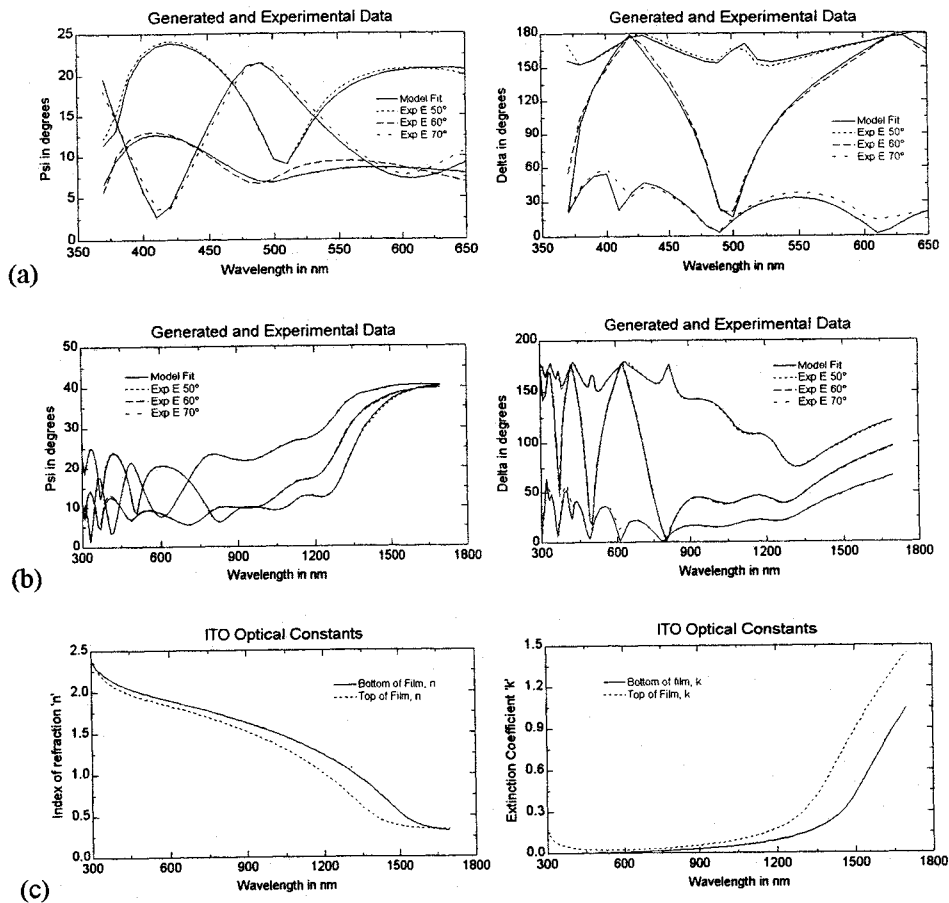


Figure 28. VASE characterization of an ITO film: (a) Data analysis using a single Cauchy film optical model results in poor data fits, even over the limited spectral range shown here. (b) A graded-film optical model (using Lorentz oscillators to model the dispersion in the ITO film) results in excellent fits to the VASE data over a wide spectral range. (c) The ITO optical constants at the top and bottom of the film are compared in this plot; the amplitude and shape of the free-carrier absorption tail (seen in the 'k' plot at the longer wavelengths) is directly related to the electrical conductivity of the film.

3.4.2. Thin-Film Transistors (TFT) Structures

Thin film transistors (TFT) are important in active matrix liquid crystal display technology. VASE can be used to characterize important TFT layer thicknesses, as shown in Figure 29. By acquiring VASE data into the NIR spectral range, the ability to characterize thicker amorphous Silicon (a-Si) films is greatly enhanced, as a-Si becomes essentially transparent in this spectral range.

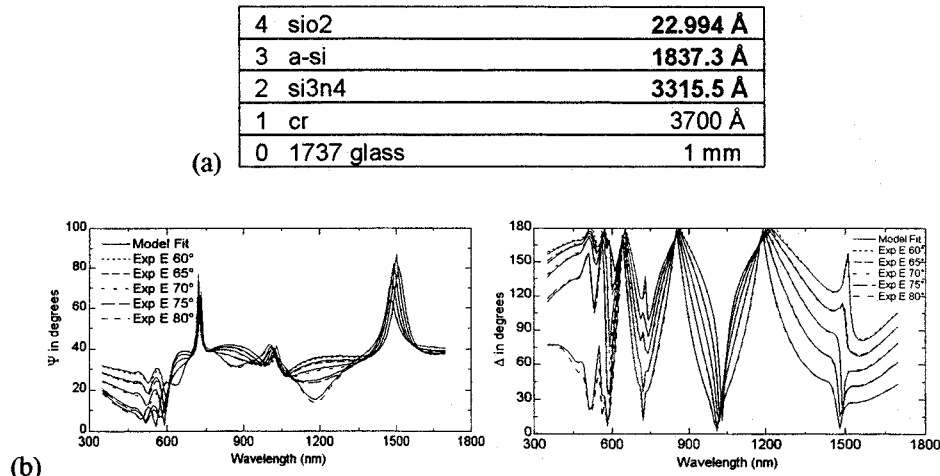


Figure 29. VASE analysis of a TFT structure: (a) optical model (only the top 3 layers were determined in this analysis, as the Cr metal layer was optically thick and therefore fixed at its nominal value), and (b) data fits.

4. AUTOMATION OF VASE MEASUREMENTS

Most of the preceding VASE examples required a time-consuming and sometimes subjective process of 'fine-tuning' the optical model to achieve acceptable data fits which accurately characterize the sample properties. However, once an appropriate optical model has been developed, it is very straightforward to apply it to the VASE data analysis of similar samples. In fact, with commercially available software, the complete VASE data acquisition and analysis procedure can be encapsulated into a recipe, such that powerful VASE metrology can be performed with the push of a button. An example of an automated VASE analysis (and reporting of extracted material parameters) is shown in Figure 30.

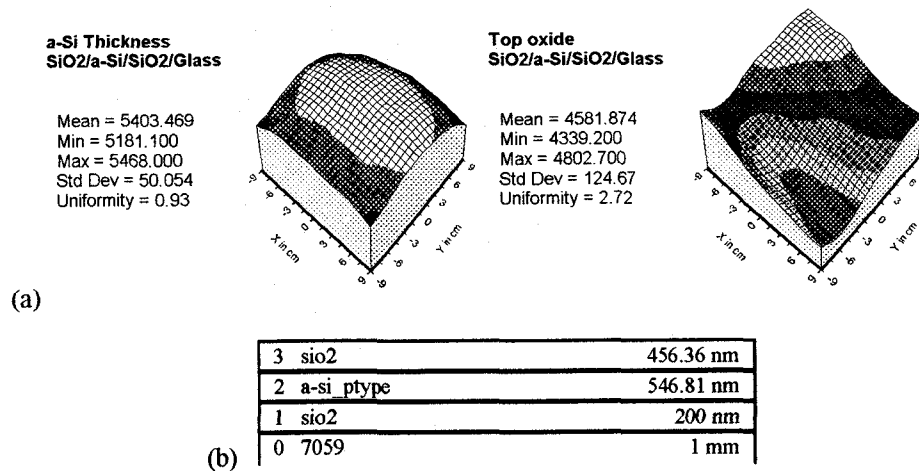


Figure 30. (a) Uniformity in layer thicknesses extracted from automated VASE measurements across the surface of a flat panel display, using the optical model shown in (b).

SUMMARY

The ability to accurately acquire and quantitatively analyze VASE data on a wide range of samples was demonstrated. Variable angle spectroscopic ellipsometry is now well-established as an important metrology tool in several different industries, and as an important technique for industrial research on new materials and processes.

ACKNOWLEDGMENTS

The authors wish to thank the many sponsors who contributed to the development of the work presented here, including NASA, BMDO, the U.S. Army and Air Force, DARPA, and numerous corporations which supplied samples.

REFERENCES

1. R.M.A. Azzam, and N.M.Bashara, Ellipsometry and Polarized Light, North Holland Press, Amsterdam 1977, Second edition 1987.
2. R.M.A.Azzam, Selected Papers on Ellipsometry, SPIE Milestone Series MS 27, 1991.
3. J.D.Jackson, Classical Electrodynamics, John Wiley & Sons, New York, 1962
4. H. G. Tompkins, and W.A.McGahan, Spectroscopic Ellipsometry and Reflectometry, John Wiley & Sons, New York, 1999.
5. A. Roseler, Infrared Spectroscopic Ellipsometry, Akademie-Verlag, Berlin, 1990.
6. Ellipsometry in the Measurement of Surfaces and Thin Films, A.Rothen, E.Passaglia, R.R.Stromberg, and J.Kruger, Natl.Bur.Std. Misc. Publ. 256, U.S. Government Printing Office, 1964.
7. Proceedings of the Symposium on Recent Developments in Ellipsometry, N.M.Bashara and A.B.Buckman, and A.C.Hall, North Holland Publishing, Amsterdam, 1969.
8. Ellipsometry, Proceedings of Third International Conference on Ellipsometry, N.M.Bashara and R.M.A. Azzam, eds, North Holland Publishing, Amsterdam, 1976.
9. Ellipsometry and other Optical Methods for Surface and Thin Film Analysis, J. de Physique, Les Ulis Cedex, FR, 1983.
10. Spectroscopic Ellipsometry, A.C.Boccara, C.Pickering, J.Rivory, eds, Elsevier Publishing, Amsterdam, 1993.
11. Spectroscopic Ellipsometry, R.W.Collins, D.E.Aspnes, and E.A. Irene, Editors, Elsevier Science S.A., 1998, Lausanne, Switzerland; also appears as Vol. 313-314 Thin Solid Films, Numbers 1-2, 1998, pp 1- 837.
12. G.H. Bu-Abbud, S.A.Alterovitz, N.M.Bashara, and J.A.Woollam, "Multiple-Wavelength-Angle-of-Incidence Ellipsometry: Application to Silicon Nitride-Gallium Arsenide Structures", J.Vac.Sci.Technol. A1, 619 (1983).
13. R.W.Collins, "Automatic rotating element ellipsometers: Calibration, Operation, and Real-time Applications", Rev.Sci.Instrum. 61, 2029 (1990).
14. W.H.Press, B.P.Flannery, S.A.Teukolsky, and W.T.Vetterling, Numerical Recipes in C, Cambridge University Press, Cambridge, 1988.
15. G.E.Jellison, Jr. "Spectroscopic ellipsometry data Analysis: Measured Versus Calculated Quantities", Thin Solid Films 313-314, 33 (1998).
16. F.Wooten, Optical Properties of Solids, Academic press, New York, 1972.
17. C.M.Herzinger, B.Johs, W.A.McGahan, and J.A.Woollam, "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, 3323 (1994).
18. B.Johs, W.A.McGahan, and J.A.Woollam, "Optical Analysis of Complex Multilayer Structures Using Multiple Data Types", Optical Interference Coatings, SPIE 2253, 107 (1994)
19. C.M.Herzinger and B.Johs, "Dielectric Function Parametric Model, and Method of Use", U.S. Patent 5,796,983, issued Aug 18, 1998.
20. R.W. Collins, I. An, H. Fujiwara, J. Lee, Y. Lu, J. Koh, and P.I. Rovira, "Advances in multichannel spectroscopic ellipsometry", Thin Solid Films 313-314, 18 (1998).
21. W.A. McGahan, B. Johs, and J.A. Woollam, "Techniques for ellipsometric measurement of the thickness and optical constants of thin absorbing films", Thin Solid Films 234, 443 (1993).
22. R.A. Synowicki, "Spectroscopic ellipsometry characterization of indium tin oxide film microstructure and optical constants", Thin Solid films 313-314, 394 (1998).
23. R.A. Synowicki, J.N. Hilfiker, R.R. Dammel, C.L. Henderson, "Refractive index measurements of photoresist and antireflective coatings with variable spectroscopic ellipsometry", Proceedings of the SPIE Vol. 3332, 384 (1998).