Measurement and Modeling of Zinc Sulfide Thin Films using Ellipsometry and Reflection Spectroscopy: A Comparison of Optical Characterization Techniques

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Abstract

Zinc sulfide thin films on silicon wafers were analyzed for layer thickness, refractive index, and absorption using reflection spectroscopy (RS), spectroscopic ellipsometry (SE), and modeling programs. RS and refractive index values from literature were used to model film thickness based on reflection and the SCOUT modeling program was used to analyze the reflectance data and generate model RS data. SE was used to measure film thickness and complex index of refraction and a VASE32 program was used to model the layers of the thin film and generate model SE data. Goals include comparing SE and RS as possible non-destructive analysis tools and developing the most efficient SCOUT interface for analyzing available optical data.

Both RS and SE data analysis have the ability to measure the thickness d and complex refractive index n and κ of ZnS given the complex refractive index of the silicon wafer. The SCOUT optical modeling software generates a graphical user interface and can analyze RS data and can be configured to analyze SE data as well.

1 Introduction

To understand how the computational model of light is generated, it is important to understand the underlying physical principles. I will begin by describing a light wave, which will give us tools to discuss specific forms of light. The electronic band structure of materials will be discussed and related to absorption. The refractive index will be discussed and used to explain reflection and refraction in a thin film. The ellipticity and polarization of light will then be explored and related to the application of polarized light in ellipsometry.

1.1 Describing Light

Light is a propogating electromagetic wave. Because the oscillating magnetic and electric field of light is coupled (this coupling is described by Maxwell's equations), only one field is needed to represent the wave. By convention, light is described by the oscillating electric field which is called the polarization. The electric field can be described by an oscillating wave propagating through space with the wave vector k and the angular frequency ω.

$$\vec{E}(\vec{r},t) = \mathrm{Re}\left[\vec{E}_0 e^{i(\vec{k}\cdot\vec{r}-\omega t)}\right] \tag{1}$$

The use of the complex phasor $e^{i\theta}$ is a mathematical tool to make computation easier. This is done knowing that we will always be taking the real part of the complex number. The wave vector is inversely proportional to the wavelength of light ($k = {}^{2\pi}/_{\lambda}$) and the angular frequency of the light is proportional to the frequency ($\omega = 2\pi f$). If we know one wavelength is λ and a peak on the wave passes a point in space with f frequency, we can say that the velocity of a point on the wave is $v = \lambda f$. It follows that

$$v = \lambda f = \left(\frac{\lambda}{2\pi}\right)(2\pi f) = \frac{\omega}{k}. \tag{2}$$

We can see that the direction of the wave is determined by the sign of the velocity, which is in determine by the relative sign of ${}^{\omega}/_{k}$ and that the speed of the wave is related to ω and k. The relation between ω and k in a medium is called the dispersion relation, and for light, is always related to the speed of the wave in the medium.

1.2 Band Structure and Absorption

All materials have a unique electronic structure that determines how the material's electrons interact with different forms of energy. Electrons in the material that are tightly bound to their parent atom are in the valence band of the material, a section of the band structure with lower energy. Electrons which are free to flow (or conduct) throughout the material are called conducting electrons and are part of the conduction band. This section of the band structure typically has higher energy than the valence band. Semiconductors can be described by the type of energy gap between the valence and conduction band: direct- and indirect-gap materials [5].

A bandstucture is a relation of the energy of an electron to its momentum. When a semiconductor exhibits a direct band gap, this means that the maximum allowable energy state in the valence band has the same momentum as the lowest allowed energy state in the conduction band. Essentially, this represents a direct peak-to-trough transition of an electron bewteen the two bands without a need to change the momentum of the particle.

An indirect band gap requires the electron change momentum to transition from the peak of the valence band to the trough of the conduction band. This momentum usually comes in the form of lattice vibrations (also known as phonons). The absportion of a material (the rate of photon absorption at a given energy) is highly dependent upon the bandgap. Only photons with energy larger than the bandgap of the material can be absorbed. When the absorption in a material is zero, the sum of the transmitted light (measured exiting the film) and the reflected light equal the light incident upon the material. When the absorption is nonzero, energy is transferred to the material and the sum of the measured transmission and reflection is no longer 1.

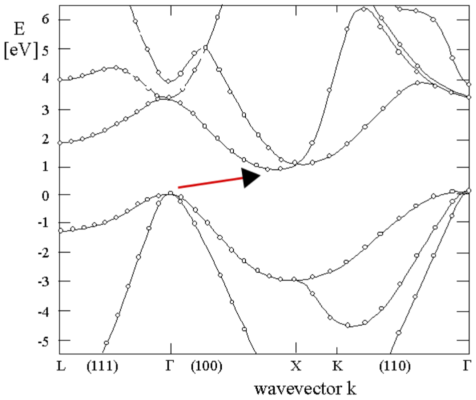


Figure 1: The band stucture of Si is shown. The indirect gap between zero and one eV represents the commonly referenced 1eV bandgap of Si. [1]

1.3 Index of Refraction

The speed of a light wave is clearly dictated by the medium through which it is travelling, however, the amplitude of the electric field can also change. If the absorption of the material is nonzero for the incident energy of light, Beer's law states that the amplitude of the electric field (and the intensity of the light) will descrease exponentially as a function of distance when travelling through the medium:

$$I(z) = I_0 e^{-\alpha(\lambda)z} \tag{3}$$

where the absorption of light travelling the the $\hat{z}$ direction in a material depends on the absorption coefficient $\alpha(\lambda)$ (which is dependent on the wavelength of the light) [2].

To describe light propagating in a material, the speed of the wave and the absorption of energy needs to be considered. In optics, the extinction coefficient κ is used to describe the absorption and is related to the absorption coefficient by

$$\alpha = \frac{4\pi\kappa}{\lambda}. \tag{4}$$

The relative velocity of the light can be described by the index of refraction $n = \frac{c_0}{v} = \frac{c_0 k}{\omega}$, where c_0 is the speed of light in a vacuum. In practice, it is common to describe both the absorption (extinction) and relavtive velocity (index of refraction) of the light in a material with a complex number, called the complex refractive index:

$$\tilde{n} = n(\lambda) + i\kappa(\lambda) \tag{5}$$

where n and κ are both wavelength dependent.

The complex refractive index of a material completely describes the optical characteristics of the material and will be used to calculate thickness of a thin film. Based on n and the interference fringes that occur in the reflectance spectrum, the thickness of a film can be calculated. Fig. 2 shows an example of these fringes. Because the film is so thin, there are fewer of the fringes than could be observed in a thicker film. The interference patterns are caused by constructive and destructive interference of reflected light at the interface. Over the range observed (0.3-0.9 μm), there are fewer maximums in the interference pattern for a thinner film because there fewer wavelengths that meet the constructive interference conditions (these conditions are discussed more in the section 1.4).

1.4 Film Reflection

Snell's Law explains how light refracts at an interface of two media. A deeper understanding of the behavior of light shows that light both reflects and refracts at an interface of two dielectric materials. Thin films most often

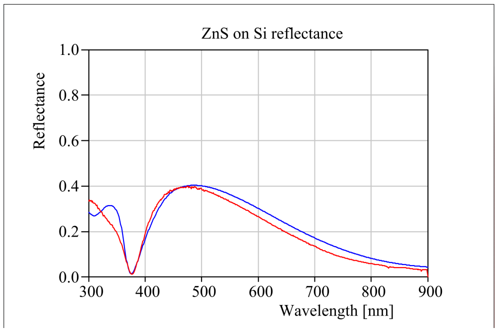
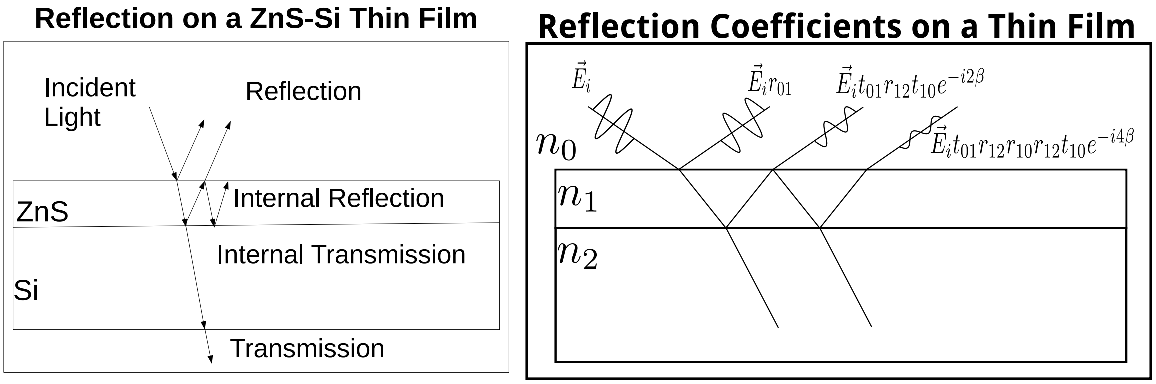


Figure 2: An example measured and SCOUT modeled spectrum from a ZnS/Si thin film. The measurement was taken over a range of 300-900nm of incident light.

are constructed on top of a substrate; this creates an interface between the two materials. There is both reflection and refraction (transmission) at this interface and at the interface of air and the top material. At each interface, part of the electric field wave reflects E_r and part transmits E_t.

Multiple interfaces create multiple reflection and transmission waves and these waves of light interfere with one another. This interference can be measured and analyzed, and this analysis can describe the thickness of the film and the refractive index. This non-destructive measurement technique is called spectroscopy and is based on classical interference equations:

$$2d = m\frac{\lambda}{n}, \qquad \text{where } \frac{\lambda}{n} \text{ is the wavelength of light inside of the material} \tag{6}$$


Reflection on a ZnS-Si Thin Film

Reflection Coefficients on a Thin Film

Figure 3: (Left) Light incident at the air-ZnS interface can both reflect and transmit. Some of the transmitted light also can bounce back from the next ZnS-Si interface and interfere with the first reflection. (Right) Reflection or transmission of light at a boundary modifies the original wave with a transmission or reflection coefficient and transmission through a medium adds phase equal to β.

At the interface of materials with indices of refraction n_i and n_j, the reflection and transmission can be calculated using the Fresnel amplitude coefficients r_{ij} and t_{ij}. The coefficients are functions of the angle of incidence and refractive index of the two materials and describe what portion of the electric field is reflected versus transmitted. Because measuring intensity of light is easier than the electric field strength, the reflectivity is often used. Reflectivity is the ratio of incident intensity to reflected intensity and is related to the reflection coefficients. Intensity is proportional to the square of the electric field, and because of the interference in the multiple reflected waves at the interface of the air and ZnS, the reflection and transmission coefficients as well as the relative phase of each reflecting electric field wave is important in calculating the total reflectivity.

$$R = \frac{|E_r|^2}{|E_i|^2} = \frac{|E_i(r_{01} + t_{01}r_{12}t_{10}e^{-i(2\beta-\gamma)} + t_{10}r_{12}r_{10}r_{12}t_{01}e^{-i(4\beta-2\gamma)} + ...)|^2}{|E_i|^2} \tag{7}$$

β is the phase difference picked up from traversing the extra distance through the thin film,

$$\beta = 2\pi\frac{nd}{\lambda cos\theta_t} \tag{8}$$

d is the film thickness, θ_t is the angle at which the light transmits through the medium, and γ is the recombination phase that each reflected beam has from exiting the material at different places

$$\gamma = \frac{4\pi d}{\lambda}tan\theta_t cos(^{\pi}/_{2} - \theta_i) \tag{9}$$

From Equation 7, it is evident that the relative phases of the reflecting electric fields is important to the intensity of the reflecting light, and depending on the wavelength, can be highly influenced by the thickness of the film and angle of incidence.

1.5 Ellipticity and Polarization of Light

In general, when light is measured, many, many photons are measured. Measurable light waves consist of many electromagnetic waves which are superimposed onto each other. Essentially, the electric fields (or polarization of each wave) are added together. At any point along the path of propagation of the light wave, the total electric field at the point is the superposition of all the existing electric fields.

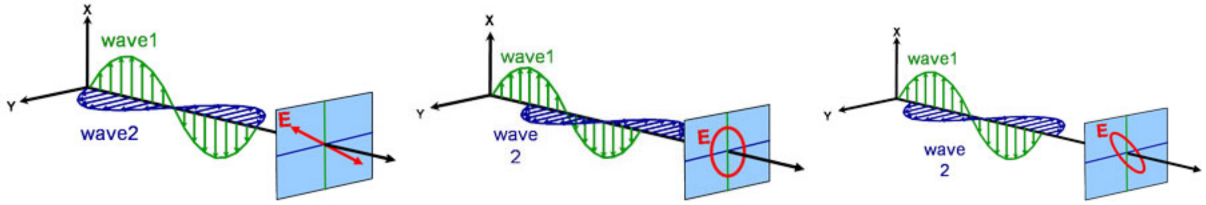


Figure 4: (*Left to right*) The superpostion of two electromagnetic waves resulting in linearly, circularly, and elliptically polarized light. [2] Light with different ratios of electric field components and different phase differences will produce differently polarized light.

Using a reverse method of vector decomposition, the incident electric field vector E_i can be broken down into orthogonal components. Because of the treatment of Maxwell's equations from the boundary conditions, the x direction, perpendicular to the direction of propagation and parallel to the plane of incidence, is useful (see Fig. 5). Choosing another orthogonal basis vector $\hat{y}$, it will be perpendicular to both the direction of propagation and the plane of incidence.

Based off of the boundary conditions and Maxwell's equations, there are separate reflection and transmission coefficients for either polarization E_x or E_y. Even though the Si wafer does not transmit at the measured wavelengths, the transmission coefficients are still included because the air-ZnS interface transmits to the ZnS layer and reflections from the ZnS-Si interface create interference that is used to calculate the thickness and refractive index of the ZnS layer. The coefficients are called the Fresnel reflection and transmission coefficients, r_x, r_y and t_x, t_y respectively, and there are a set of coefficients for every interface.

Assuming that the permeability of the materials μ_1, μ_2 in the sample is equal to the permeability of free space

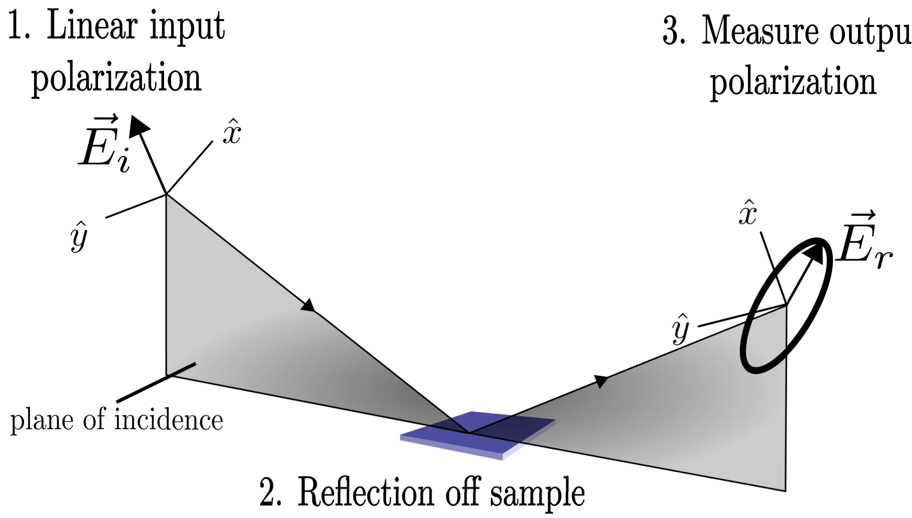


Figure 5: General ellipsometry experiment. 1. Linearly polarized light is incident upon the sample. 2. [2]

μ_0 (which is approximately true for ZnS and other dielectrics), the Fresnel coefficients are: [3]

$$r_x \equiv \left(\frac{E_{0r}}{E_{0i}}\right)_x = \left(\frac{n_t cos\theta_i - n_i cos\theta_t}{n_t cos\theta_i + n_i cos\theta_t}\right) \qquad r_y \equiv \left(\frac{E_{0r}}{E_{0i}}\right)_y = \left(\frac{n_t cos\theta_i - n_i cos\theta_t}{n_t cos\theta_i + n_i cos\theta_t}\right) \tag{10}$$

$$t_x \equiv \left(\frac{E_{0t}}{E_{0i}}\right)_x = \left(\frac{n_t cos\theta_i - n_i cos\theta_t}{n_t cos\theta_i + n_i cos\theta_t}\right) \qquad t_y \equiv \left(\frac{E_{0t}}{E_{0i}}\right)_y = \left(\frac{n_t cos\theta_i - n_i cos\theta_t}{n_t cos\theta_i + n_i cos\theta_t}\right) \tag{11}$$

2 Methods

2.1 Ellipsometry

Ellipsometry is also a non-destructive technique that is used to characterize materials. It uses the change in polarization of light after reflection to calculate the refractive index and thickness of a material.

Because light is made up of electric and magnetic fields, both of which are vector fields, light can be decomposed into component vector polarizations. After light reflects from a material, the polarization of the wave has changed, which means the relative strengths of the component electric fields have changed or there is a phase difference between them. The complex reflection coefficients $\tilde{r}$ give the reflected electric field components in terms of the incident electric field:

$$\vec{E}_{rx} = \tilde{r}_x \vec{E}_{ix} \qquad \vec{E}_{ry} = \tilde{r}_y \vec{E}_{iy} \tag{12}$$

Assuming the incident light is linearly polarized (both electric field components are in phase), the ratio of the complex reflection coefficients gives the ratio of the reflected electric field strengths and the relative phase between them. Ψ and Δ are used to describe the strength ratio and phase difference, respectively:

$$tan\Psi e^{i\Delta} = \frac{\tilde{r}_x}{\tilde{r}_y} = \frac{\vec{E}_{rx}/\vec{E}_{ix}}{\vec{E}_{ry}/\vec{E}_{iy}} = \frac{E_{rx0}/E_{ixo} e^{i\phi_r x}}{E_{ry0}/E_{iy0} e^{i\phi_r y}} \tag{13}$$

$$tan\Psi = \frac{E_{rx0}/E_{ixo}}{E_{ry0}/E_{iy0}} \qquad e^{i\Delta} = e^{i(\phi_r x - \phi_r y)} \tag{14}$$

ϕ_{rx} and ϕ_{ry} are the phases of the reflected x and y components of the electric field, relative to the incident electric field.

In an ellipsometry experiment, the measurable quantities are the incident and reflected light intensities, which are proportional to the electric fields squared, E^2. Using polarizers and phase modulators, the magnitude of the electric field components, as well as their relative phase can be calculated from the intensities for both the incident and reflected waves.

Based on a model's n and κ, Ψ and Δ are generated for the range of wavelengths used and compared to the measured values. The values of n and κ and altered to provide a best fit of the model's Ψ and Δ.

2.2 McIntyre Grating Spectroscopy

2.2.1 Experiment Overview

Figure 6 shows a simplified version of the McIntyre lab grating spectrometer setup. 300-900 nm light (ranging from near ultraviolet to infrared) exits the Xe lamp source. This polychromatic (multiple wavelength) light, is then filtered using two series grating monochromators. Grating monochromators use gratings to reflect light at different angles depending on the wavelength. The grating can then be rotated to allow only a small range of wavelengths to pass through a small opening in the side. This opening leads to another monochromator which again filters the light so the light out of second monochromator has a very narrow band of wavelengths. This light is considered experimentally close to monochromatic light (light containing only one wavelength) and has a wavelength band narrow enough to allow for the appropriate calculations of reflectance and transmittance. The monochromatic light is then reflected off the sample and back into the silicon (Si) detector for reflection measurements and the transmission is negligible for films on Si wafers. The angle of incidence is about 10 degrees from normal, which is approximated as normal in most calculations.

2.2.2 Details About Procedure

Because the intensity of the Xe lamp light source changes while warming up, it is important to give it at least 20 minutes to warm up and level off. Reflectance and transmission are relative values and represent a ratio of the reflected intensity from the film to the incident intensity from the lamp. Because the setup does not include a reliable method for splitting the beam two, with equal intensity, the incident intensity for each wavelength must be measured separately from the reflection measurements. Allowing the lamp time to warm up and level off in intensity is important because the original lamp spectrum measurement would underestimate the incident intensities during the rest of the experiment and would throw off the ratio of reflected light to incident light.

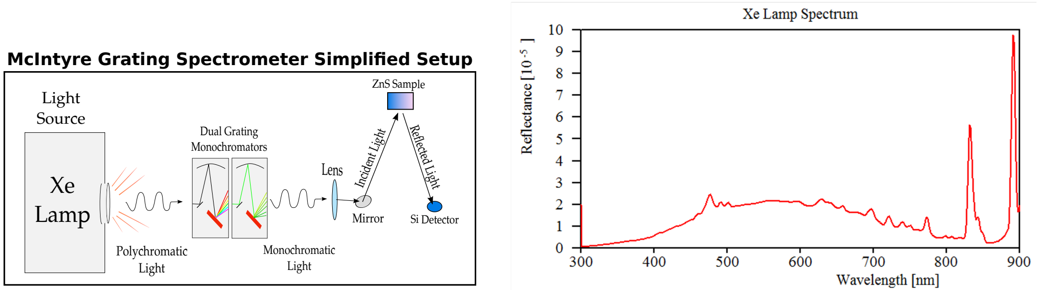


Figure 6: (left) A simplified experimental setup of the McIntyre lab grating spectrometer setup. In practice, there are more mirrors, lenses, and irises used to guide and focus the beam. (right) The Xe lamp spectrum, which includes the visible range.

2.3 VASE32 Ellipsometry Equipment

The VASE32 spectroscopic ellipsometer uses five specific incident polarizations of light and measures polarization change after reflection:

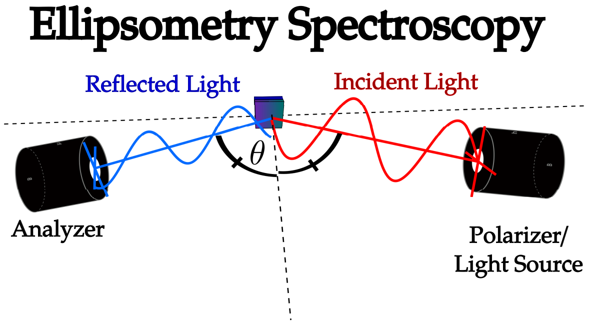


Figure 7: The general setup for ellipsometry includes a source of light with known polarization and an analyzer which can measure the phase and the polarization of the light reflected from the film.

2.3.1 Ellipsometry Setup

The ellipsometer uses a Xe lamp which supplies light in a range of 193 to 3200 nm, but the fiber optic cable that is used to guide the light to the measurement stage of the ellipsometer is optimized for 300 to 2300 nm. Once the lamp warms up for about 20 minutes, light in the 300 to 2300 nm range is steady in intensity, and only fluctuates in a few percentage points of the intensity of the beam. The main part of the incident beam measures about 1 mm in diameter.

The angle of incidence θ in Fig. 7 can be changed to give more detailed data and allow for a better fit. Generally, three different angles are chosen and data is collected for each incident angle. The common incident angles chosen are $\theta = 65, 70,$ and $75°$.

2.3.2 Ellipsometry Experiment

It is important to keep the optical cables as still as possible during the entire experiment. If the cables are nudged, the intensity of the light changes because different bends in the cable result in a different effective optical impedance. This can affect the measurements being taken during the experiment and result in false features in the data and an inaccurate model fitted to the data.

Optical experiments require a steady, reliable light source from experiment to experiment so it is also important to monitor different qualities of the produced light each time data is acquired. An intensity profile (intensity as a function of wavelength) of the lamp should be recorded to ensure that results from different experiments are comparable. As in the McIntyre grating spectrometer setup, the lamp used in the ellipsometry setup requires time to warm up and the intensity to level off. This generally takes about 20 minutes and can be monitored by engaging the intensity measurement tools in the ellipsometry interface.

After the lamp intensity levels off, the calibrations can be made on a large, clean Si wafer. The VASE software has pre-programmed ellipsometry data (see sect. 2.1) for a reference Si wafer, which has been thoroughly verified in the ellipsometry literature. The ellipsometry device measures the reflected light from the Si wafer and compares the data to the reference data to make the proper calibrations of the equipment. The experimental sample is then mounted and the plane of the sample film is finely adjusted to maximize the intensity being measured (Fig. 8). This ensures that the signal-to-noise ratio is largest by changing subtle tilt angles of the film to allow the most reflected light to hit the detector. The tilt angles need to be adjusted for every sample because the substrate may be different size or the film surface may be at a slight angle.

Because the film surfaces are not always uniform, we may want to focus the measurement on a specific part of the film. The sample stage (where the sample is mounted) can be adjusted in two orthogonal directions during normal incidence to allow the beam to be focused on a specific part of the film. Setting up to this point takes

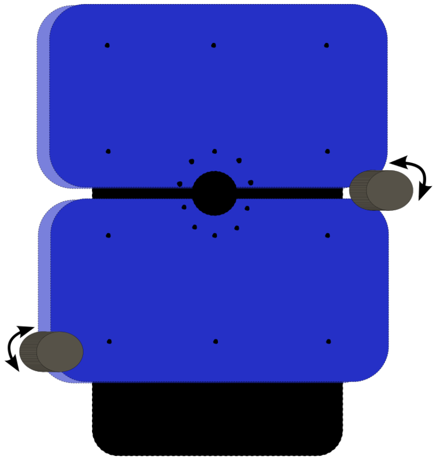


Figure 8: Knobs on the measurement stage of the VASE32 ellipsometry equipment adjust the subtle tilt angles of the plane of the sample film. The small holes in the face of the stage are connected to vacuum to keep the film vertical on the stage.

about 30-40 minutes on average.

There types of scans possible depending on the detail of the data needed. The short scan consists of a small set of ellipsometric data (polarization and phase changes after reflection), which can be used to model the thickness of the film. This scan generally uses one type of incident polarization, starts at one angle of incidence and sweeps through the desired range of wavelengths before changing the angle of incidence and sweeping again. This portion of the experiment takes about 30-50 minutes, depending on the range of wavelengths and the distance between each measured wavelength.

A longer scan can be completed which uses multiple polarizations to gather more detailed information. This method uses up to five different polarizations, determined by the user, and can be used to model-fit the index of refraction of the film, as well as the thickness. The angle of incidence is set, then the monochromator changes the incident light to the desired wavelength (for a description of the monochromator, see Section 2.2.1. The polarizer then changes the incident polarization (through the five different polarizations) while the analyzer reads the reflected phase and polarization. Then the monochromator shifts to the next wavelength in the data set, and the polarization scan is repeated. This is repeated for all wavelengths in the set, then the entire wavelength scan is repeated for each incident angle. This portion of the experiment can take upto 1.5 hours, but produces more detailed and verifiable data.

The longer scan is being used for the current data collection because there is a second layer of verification of the quality of the film. The longer scan fits a model refractive index to the data to determine an experimental refractive index of the film. The experimental refractive index can be compared to the theoretical refractive index of the material, and if there is a large difference between the indicies, that can indicate an impurity or a defect in the film or an issue with the model.

2.3.3 Ellipsometry Modeling

The model polarization ratio Ψ and phase difference Δ can be calculated given guess thicknesses of the materials in the layer stack and a model of their refractive indices at each wavelength. This model can be compared to the actual data and the thicknesses and refractive indices of layers can be changed as parameters to best fit the model Ψ and Δ. The model is changed until the error is minimized.

$$\text{MEAN-SQUARED ERROR:} \quad \text{MSE} = \sqrt{\frac{1}{2N-M}\sum_{i=1}^{N}\left[\left(\frac{\Psi_i^{mod}-\Psi_i^{exp}}{\sigma^{exp}(\Psi_i)}\right)^2+\left(\frac{\Delta_i^{mod}-\Delta_i^{exp}}{\sigma^{exp}(\Delta_i)}\right)^2\right]} \tag{15}$$

Not all local minima that the VASE program finds are the global minima, but because Ψ and Δ are sensitive to both thickness and refractive index, the model is noticeably unmatched to the data if it is not the global minimum. Figures 11 and 12 are an example of how close the model is to the experimental data at a global error minimum.

The VASE program uses the Cauchy refractive index model, which assumes no absorption in a large portion of the data.

$$\text{Cauchy Refractive Index Model: } n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} \tag{16}$$

Rather than adjusting the refractive index at each wavelength, it can be assumed that the refractive index is a smooth function of wavelength and decreases in regions without absorption as wavelength increases. Adjusting the model parameters (A, B, C and the ZnS film thickness d) to decrease the error between the model and the data allows the user to fit the data and find the experimental refractive index and film thickness at the point of reflection.

2.4 Other Methods in literature

Lazarova et. al. use an oscillator model to describe the complex refractive index $\tilde{n} = n + i\kappa$,

$$n(E) = \sqrt{1 + \frac{E_0 E_d}{E_0^2 - E^2}}, \quad \alpha(E) = a_0 e^{E/A}, \quad \kappa = \frac{\alpha\lambda}{4\pi} \tag{17}$$

where they use E_0, E_d, a, and A as modeling “parameters that are constants in the whole spectral range” [4].

2.5 SCOUT Data Analysis Software

The SCOUT optical analysis software interface is in the process of development. Ultimately, SCOUT will be used to compare ellipsometry and spectroscopy data. Fig. 13 is an example of an interface that displays measured and modeled reflectance data from the McIntyre grating spectrometer. SCOUT offers a mathematical optimization algorithm to fit the model to the measurement.

2.5.1 Fitting

The optimization process is a minimization of the error between the model and experimental reflectance curves.

$$\text{MEAN-SQUARED ERROR:} \quad \text{MSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(R_{exp}(\lambda_i) - R_{mod}(\lambda_i)\right)^2} \tag{18}$$

The SCOUT program has the flexibility to use many different characteristics of the optical model as the parameters to fit the model to the data. A ’model parameter’ is a piece of the optical model (index of refraction, carrier mobility, surface roughness, layer thickness) that can be changed manually to change the calculated reflectance. ’Fit parameters’ refer to the model parameters which are automatically tuned by the program during the fitting process to minimize the error. In its current configuration, the index of refraction and the ZnS film thickness are fit parameters, while a surface silicon dioxide layer thickness is a model parameter that can be changes manually, but not during the fitting optimization process.

Taking into account the limitations of our system and model, it is possible that the experimental data should be narrowed to allow for a better fit. One common issue arises because of the low strength of the incident light at low wavelengths. The Xe lamp that is used in some experiments is a less reliable light source below 400 nm. Because the incident intensity below 400 nm might fluctuate during the experiment, the data may need to be trimmed to exclude the less-reliable data. Changing the fitting range from 300-900 nm to 400-900 nm can improve the error estimation and increase the accuracy of the model.

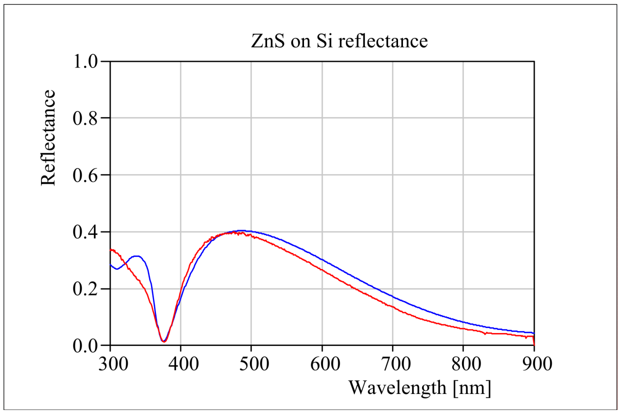


Figure 9: An example of a SCOUT generated model and experimental data of a ZnS thin film. The red experimentally measured and the blue data is theoretically generated using SCOUT. Note the non-ideal feature occurring between 300 and 400 nm.

The model film thickness is changed (which changes the entire model curve, generally shifting the peaks and troughs) to minimize the area between the curves. Because matching the interference patterns involves matching the peaks and troughs of the fit to the data, the model might have to be manually adjusted depending on which peaks and troughs are more reliable.

In this case, the lamp spectrum is falling off in intensity and becomes unstable below 350 nm. This indicates that we should take into account the critical points of the graph that fall into larger wavelengths and weigh them greater than the features occurring below 350 nm for this life.

3 Results

Results from the McIntyre reflection and the Dearborne ellipsometry experimental stations using a ZnS thin film on a Si wafer are shown below.

3.1 McIntyre Grating Spectroscopy

Reflectance spectra can be used to calculate the complex refractive index and the thickness of the material. These calculations require some assumptions about the material, however.

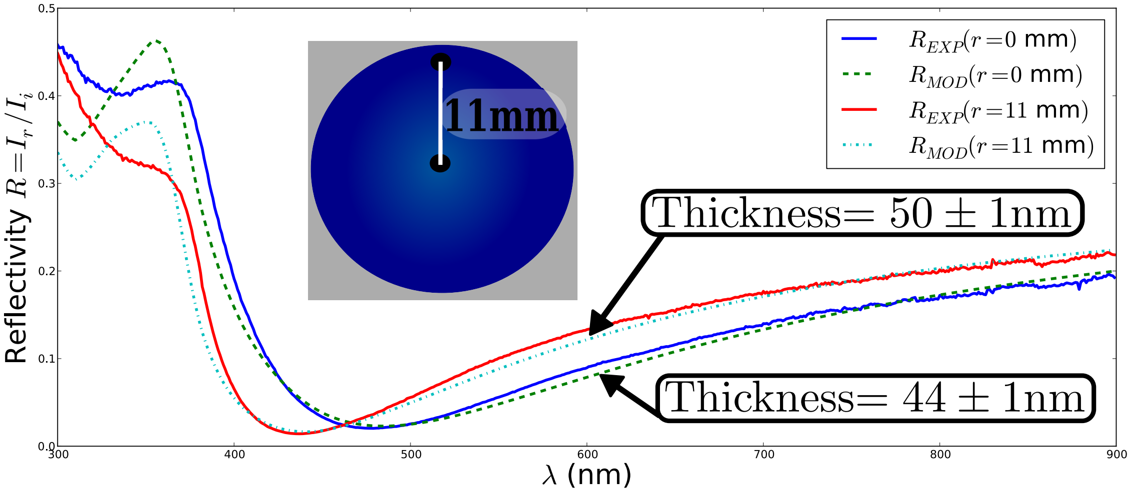


Figure 10: An example of a SCOUT reflectance model fit that is only based on the thickness of the ZnS thin film layer. The refractive index of the ZnS layer is assumed to be the same as bulk ZnS.

3.2 VASE32 Ellipsometry Equipment

The VASE32 spectroscopic ellipsometer uses five different incident polarizations of light and measures polarization change after reflection:

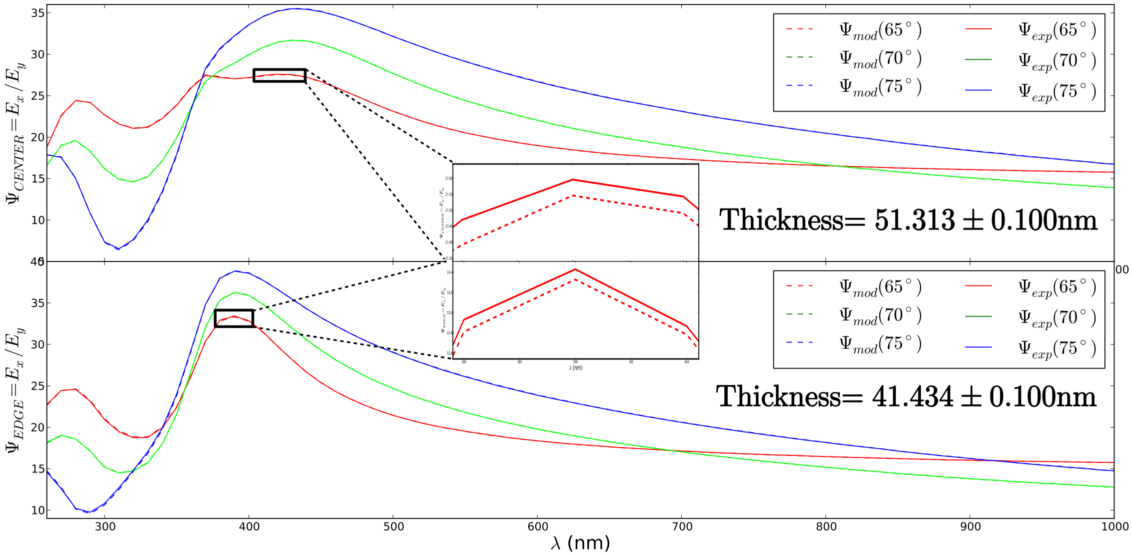


Figure 11: Ψ data and film model for an analysis of the center and edge of a ZnS thin film.

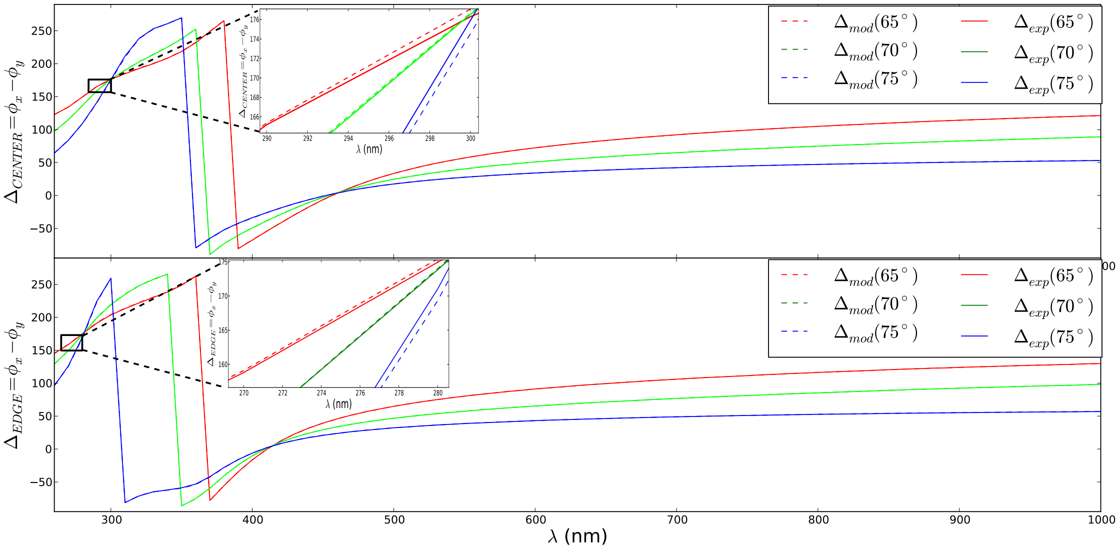
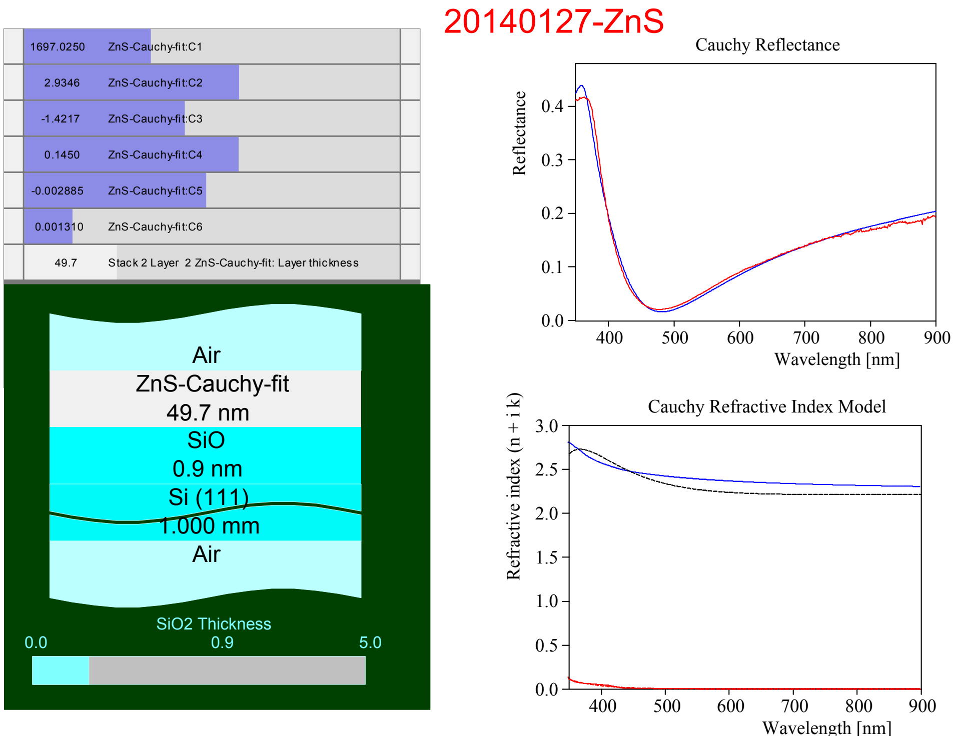


Figure 12: Δ data and film model for an analysis of the center and edge of a ZnS thin film.

3.3 SCOUT Data Analysis Software



1697.0250 ZnS-Cauchy-fit:C1
2.9346 ZnS-Cauchy-fit:C2
-1.4217 ZnS-Cauchy-fit:C3
0.1450 ZnS-Cauchy-fit:C4
-0.002885 ZnS-Cauchy-fit:C5
0.001310 ZnS-Cauchy-fit:C6
49.7 Stack 2 Layer 2 ZnS-Cauchy-fit: Layer thickness

Figure 13: SCOUT, an R/T data analysis program, optimized an optical model to fit the data. The reflectance data and fitted model reflectance (top right), the bulk and model refractive indices (bottom right), the model parameters (top left) and a visual representation of the layers (bottom left) are given as output.

In Figure 13, the Cauchy refractive index model has 5 parameters that can be controlled manually with horizontal sliders in the top left of the graphical interface. Once the user manually changes the parameters to match the model reflectance to the data, the error minimization process and be started and the model parameters will be finely adjusted to minimize the difference between the model reflectance and the data.

The bottom right of Figure 13 compares the model refractive index (black) and the bulk ZnS refractive index from the SOPRA database (blue). The red lines near the bottom of the graph are the imaginary components of the refractive index, which are related to absorption. Because the SOPRA values indicated a small amount of absorption between 300-450nm, the imaginary component of the model refractive index was manually adjusted to include the same amount of absorption.

4 Discussion

4.1 Multiple Error Minimums in SCOUT

The VASE32 ellipsometry equipment generally generates six different data points per wavelength (Ψ and Δ at three different angles of incidence). This makes finding the global minimum much easier because the different angles of incidence make changes in the film thickness unique. Ψ and Δ are more sensitive to changes in index of refraction than the reflectance measurements, which makes it easier to graphically define the error minimum (looking at the Ψ and Δ data and model and seeing the differences between them). The grating spectrometer reflectance setup only produces one data point per wavelength, which makes it difficult to graphically discern the best fit. This is because there can be multiple pairs of refractive index models and film thicknesses that produce nearly the same reflectance curve.

Two data points per wavelength would be possible for the grating spectroscopy setup if materials that transmitted light were used. Because the shape of the transmission changes differently with changes in refractive index from the reflectivity ($T \propto n^2$, whereas $R \propto n^2 + n + c$), the minimums in error will be more unique, and the results will be more reliable.

4.2 Characterizing ZnS Thin Films

Two different samples of ZnS were used for these results. There is not significant data to conclude any interesting behavior about the ZnS thin films, but more ZnS samples that range in thickness could be used to understand how the thickness effects the refractive index.

4.3 SCOUT's Next Steps

The SCOUT interface is very useful for people who know how to use the program. However, it has not been fully developed to allow users to only interact with the user interface. In order to add experimental data and change the layers, the user must be able to use the background programming interface. The next step is to create a user interface that can be used from start to finish without needing to access the background interface.

SCOUT can handle various types of optical data, one of which being ellipsometric data. Adding a configuration that fits the ellipsometric data would allow for direct comparison of accuracy between ellipsometry and reflectance spectroscopy. Modifying the existing configuration to fit the ellipsometric data alongside the reflectance data would allow for the most accurate generation of the thickness and refractive index of the material.

References

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