Angular Spectrum Approach to Optical Characterization of Thin Film Materials Using Transmission Spectroscopy

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Abstract: Thin film transmission spectroscopy systems are useful for characterizing semiconductors, but often rely on rigid analytical models. We introduce a more versatile framework using angular spectrum diffraction, which allows for accurate characterization of inhomogenous materials.

Keywords: transmission spectroscopy, thin film, angular spectrum method, simulation, inverse synthesis, optimization

1. Introduction

Semiconductor thin films are an important component in solar panels and other photonic devices. To be properly integrated into a design, their optical properties (such as the index of refraction and extinction coefficients) must be precisely measured. This is done with different forms of thin film spectroscopy. The most common method of performing thin film spectroscopy is ellipsometry [1]. Transmission spectroscopy [2] stands out as a promising alternative due to its relatively low hardware cost and low complexity. In addition, transmission spectrophotometers are already widely available, largely due to their prevalent use in analyzing cuvette samples in chemistry and biology. Moreover, it has been shown that transmission spectroscopy can even outperform ellipsometry analyses in the spectral region of medium to weak film absorption [3]. Because most of the light is transmitted, the results of transmission spectroscopy rely more on the volumetric properties of a film than its surface properties.

In this contribution, we will show a new method of processing transmission spectrophotometer data to recover optical properties, which can potentially allow for the characterization of unusual or inhomogenous samples.

2. Background

Transmission spectroscopy is performed by measuring the transmission spectrum of a thin film, then deriving the refractive index and extinction coefficient spectra of the film from this information. A schematic of a standard system is shown in Figure 1. A partially coherent illumination system emits light at a broad spectrum (typically between 300 and 2500 nm) which is transmitted through the sample. To measure the transmission spectrum, the spectrophotometer slowly shifts through the measured wavelengths and records the respective measured intensities. By taking intensity measurements without the thin film present, enough information is obtained to calculate a transmission spectrum. From this spectrum, the optical properties of the film can be found via multiple procedures. The most important methods are inverse synthesis methods [4], which model the response of a thin film system with a set of analytical expressions, and then optimize the model to fit the measured transmission data to calculated transmission data. Once the fit is complete, refractive indices and extinction coefficients of a film can be determined from the optimized model inputs.

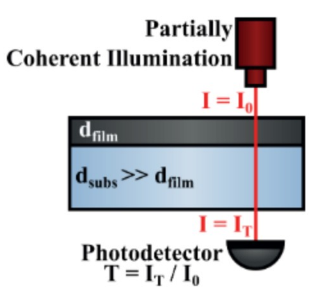

Figure 1: Schematic of Transmission Spectroscopy System

Inverse synthesis methods currently produce the most precise measurement results for transmission spectroscopy, but still suffer from several drawbacks: Since they rely on analytial expressions, they typically only work on well-prepared samples. In cases of beam tilt, surface tilt, or refractive index inhomogeneity, these methods can produce poor fits which can lead to wrong characterization results. A novel method that accounts for these effects could significantly improve characterization quality and would even allow for the characterization of "exotic" samples which are hard to describe with an analytical model.

3. Methods

We developed a new method of inverse synthesis to precisely characterize imperfectly prepared thin film systems. Our method works as follows: First, we simulate a thin film under test using a novel simulation method based on split-step angular spectrum diffraction. This produces a transmission spectrum that could be produced by a real thin-film system. Next, we compare this simulated spectrum to a real, measured transmission spectrum taken by a spectrophotometer of our thin film sample. If the simulated spectrum does not closely match the measured spectrum, we repeat the simulation with slightly different inputs to a material model for the thin film. The simulation now produces a new transmission spectrum assuming slightly different thin film optical properties, which we once again compare to a measured spectrum. Repeating this process while optimizing the material inputs along the way will eventually produce a transmis-

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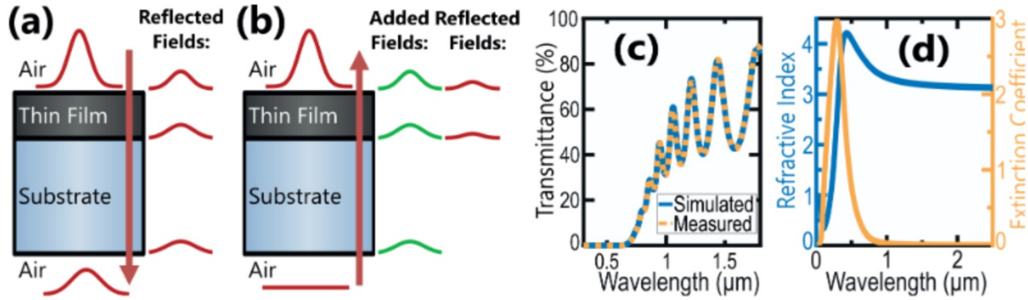

Figure 2: (a) Schematic explanation of forward propagation. The simulator propagates a gaussian beam through a thin film system, with reflections saved along the way. (b) An empty beam is then reverse propagated, adding reflected light at every step and saving new reflections. (c) Optimized simulated transmission spectrum of amorphous silicon, as compared to a measured spectrum. (d) Measurement of optical properties of amorphous silicon, produced by our method.

sion spectrum that is extremely close to reality. Then, using the optimized material model parameters, we can generate spectra for the refractive index and extinction coefficient that accurately describe our sample.

To accomplish this method, we developed a simulator that uses a split-step angular spectrum method to precisely simulate the transmission and reflection spectra of a thin-film system. We then developed an optimization routine that finds the material properties of a thin film by comparing simulated transmission spectra to measured results. In the following paragraphs, we will explain the details of our algorithm.

Our simulator is based on the hybrid angular spectrum method [5]. We represent a thin film spectroscopy system as a set of four uniform media: air, then a thin film, then a glass substrate that the film rests on, then air. We assume that a gaussian beam is sent into the system, then propagate through each medium in order, storing reflected fields along the way, as shown in Fig. 2(a). Once this is complete, we perform a reverse propagation with a similar principle. We start with a field with zero light, then add existing reflected fields and save new reflections, as shown in Fig. 2(b). We continue propagating in both directions until newly reflected fields have less than -30dB of the original field power. By summing and integrating the propagated fields on each side, we obtain the transmittance and reflectance of a thin film system for one wavelength. We repeat this simulation for many wavelengths to get full transmittance and reflectance spectra.

We used a single oscillator Tauch-Urbach-Lorentz model [6] to model the dispersive properties of the thin film. This allows us to generate full transmittance spectra from a set of few material model inputs. We optimize the inputs of this model to characterize the optical properties of the thin film. To perform this optimization, we use gradient descent to find the set of material model inputs that minimize the root squared mean error (RSME) between the simulated and measured ground truth transmittance spectra. Once optimization is complete, we should have a set of material model inputs that precisely characterize our thin film and produce accurate refractive indices and extinction coefficients for any wavelength.

4. Results and Conclusion

To validate our proposed method, we conducted spectral analysis on the transmission data taken from the amorphous silicon sample previously characterized and discussed in [7]. After performing optimization with our novel simulator, we achieved a fit of the sample's transmission function with an RSME of 0.65%. The simulated transmission spectrum of our simulator after the fit, as compared to the measured spectrum, is depicted in Figure 2(c). The optical properties for the silicon sample, derived from these properties, are shown in Figure 2(d). Our fit produces comparable performance to state-of-the-art methods (an RSME of 0.56% was demonstrated in [7] for this sample) demonstrating that the simulator functions correctly for well-prepared materials. In addition, it incorporates functionality that could produce strong fits for imperfectly-prepared materials. These results indicate that the the angular spectrum method is a feasible method for producing inverse-synthesis based transmission spectroscopy measurements of semiconductor thin films. In future work, we want to develop this method further to allow characterization inhomogenous thin films, by accounting for surface curvature and index inhomogeneity inside the thin film.

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