Spectrometer Data Analysis For Silicon Oxide Thickness Measurement

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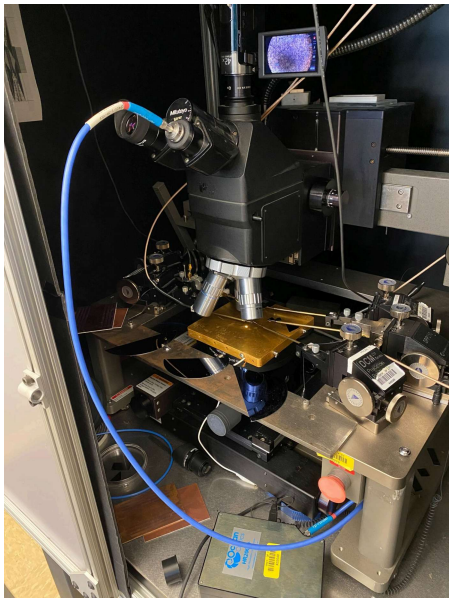
Abstract

Information regarding the thickness of Silicon Oxide on a wafer can be particularly helpful in understanding the performance of the semiconductor under different conditions. The thickness of the Oxide can determine its dielectric characteristics, anti-contamination properties, masking capabilities, and isolation potential. Controlled and measurable Oxide layers result in desirable characteristics and consistent performance. Measuring the thickness of these wafers is virtually impossible using linear measurement instruments, and so it is critical to find a method of measurement that is both reliable and unobtrusive to the fragile nature of the Oxide layer.

When Silicon wafers develop an Oxide layer, they begin to exhibit thin film optical interference. This phenomenon, when light reflects both off the oxide and the underlying Silicon layer, results in an apparent color as a function of the thickness of the Oxide layer. Using a high resolution spectrum analyzer such as the Ocean Optics HR2000+, we are able to measure the emitted wavelengths of light within .2nm, and mathematically should be able to calculate the thickness of the Silicon Oxide within a few nanometers error using least square optimization.

The other common optical method of calculating the thickness of Silicon Oxide is the use of the Fast Fourier Transform. When the Oxide layer is thick, the spectra exhibits fringe cycles- repeating patterns of wavelengths that can be measured to determine which stage, and thus which thickness the oxide layer is. However, our use case is initially with that of thin Silicon Oxide (1-200nm) which is too thin to produce a repeating fringe cycle. This makes the FFT a very poor tool for this task, and thus it is best left to the least square optimization of our model to approximate the thickness. However, as a result this model will not work for thicker oxide layers, and instead an FFT may be the preferred method of determining Oxide width.



The Spectrometer

The Ocean Optics HR2000+ in our configuration has its optical fiber and coupling fitted to a specialized 3D part that places it precisely in the center of a microscope eyepiece tube. This allows us to isolate the light entering the spectrometer to that emitted by our full spectrum, tungsten halogen lightsource, allowing intensity response to a wide range of wavelengths to be observed.

To get the reflectance of the sample which is both dependent on wavelength and SiO_2 thickness, we need to be able to filter out a very heavy, wavelength dependent noise coefficient represented as $S(\boldsymbol{\lambda})$ that alters the intensity received by the spectrometer. This coefficient dependent on wavelength, fiberoptic coupling, light intensity, and other external factors is virtually impossible to characterize, and so it is easier to take a reference measurement with the exact same setup prior to collecting data on the sample, so that we can divide out the noise coefficient and then normalize the sample's reflectance against the reference.

$$I_{sample} = S(\boldsymbol{\lambda}) * R_{sample}$$
$$I_{Si} = S(\boldsymbol{\lambda}) * R_{Si}$$
$$I_{sample}/I_{si} = R_{sample}/R_{Si}$$
$$(R_{sample}/R_{Si}) * R_{Si} = R_{sample}$$

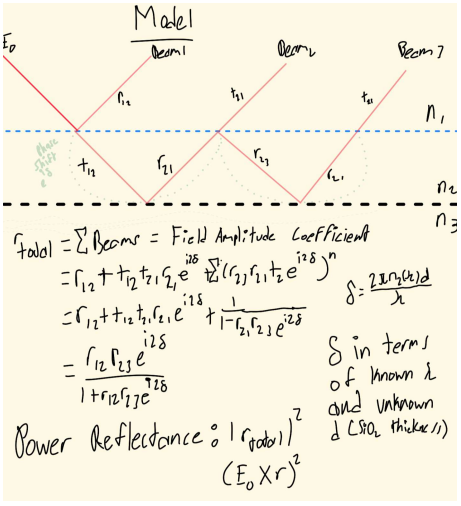
Finally, it is important that before dividing our samples, we subtract dark measurements. These measurements, taken in ambient light with the bulb on but microscope closed, allows the spectrometer to pick up on the light levels at its "darkest", and subtracting this is like zeroing a scale before weighing an object. Subtracting dark measurements from both the sample and the reference is crucial to getting a good result.

The Model

After procuring a sample reflectance graph that is (ideally) only a function of known wavelength and an unknown Silicon Oxide thickness, we can use wave-optics to produce a model that can represent any graph, with any number of wavelengths and any number of SiO_2 thicknesses. To produce this model, let us assume our Silicon sheet is semi-infinite as Silicon has high absorption and will in our cases always be large enough that light will not reflect off its back surface. Assuming this, we can model the SiO_2 as a thin film and use Fresnel equations to describe the light being transmitted and reflected from the film.

By assuming an arbitrary beam intensity E_0, we can find the total amplitude reflectance coefficient r_{total} that will be picked up by the photodetectors. The reflectance of the sample, as described by Fresnel, is $|r_{total}|^2$. Thus, if we are able to generate an accurate model that provides us with r_{total}, we will be able to create a model that matches our measured spectrometer data.

The model for r_{total} has been derived and is depicted below.



The Program

Our spectrometer intensity data is put in an array indexed by wavelength. Then, our model is run at each indexed wavelength, and tries to minimize the error between itself and the measured data by running a bounded minimization function. The bounds are values of d, the thickness of the model Silicon Oxide. The model does this for each wavelength, and determines which value of Silicon Oxide produces the least amount of error in the model and is thus closest to the real value of the SiO_2 thickness.

The model, as you may have noticed prior, depends on the indices of refraction for our 3 mediums. Air is quite simple, and is modeled as 1.0003, while SiO_2 is complicated and Si is even more so. Both SiO_2 and Si have indices which are wavelength dependent and thus, it is important to calculate these for every case rather than just use a general value. SiO_2 is less complicated to implement, as there are already very well documented coefficients for the Sellmeier equation which offers very accurate wavelength dependent indices. Si on the other hand, is slightly annoying to implement due to its complex index which accounts for its high absorption. With complex numbers being slightly difficult to compute in a large equation, a simpler and still highly accurate solution was to take a linear approximation of the real component, the complex component and add them together. There are well documented charts of hundreds upon hundreds of measurements of Silicon's index in its particular components and so by inserting 400 data points for the real and 400 for the complex, a linear approximation finds a close enough answer for high resolution results. More data points can be added should even more precise measurement be required.

$$n^2 - 1 = \frac{0.6961663\lambda^2}{\lambda^2 - 0.0684043^2} + \frac{0.4079426\lambda^2}{\lambda^2 - 0.1162414^2} + \frac{0.8974794\lambda^2}{\lambda^2 - 9.896161^2}$$

(Left) Sellmeier Equation

The program currently is limited to whatever bounds are currently input into the physical code, so if the bounds are [1,300], the model cannot return a thickness less than 1nm or greater than 300nm, even if they would offer lesser error. This is important because SiO_2 repeats fringe patterns which can confuse the model when trying to fit a curve to it as the curves mimic one another. To address this issue and avoid needing to manually change the bounds every time there is a larger or smaller sample, a future FFT will be introduced which can determine in what ~100nm range the SiO_2 thickness is, and then the model will be applied to get stronger resolution.

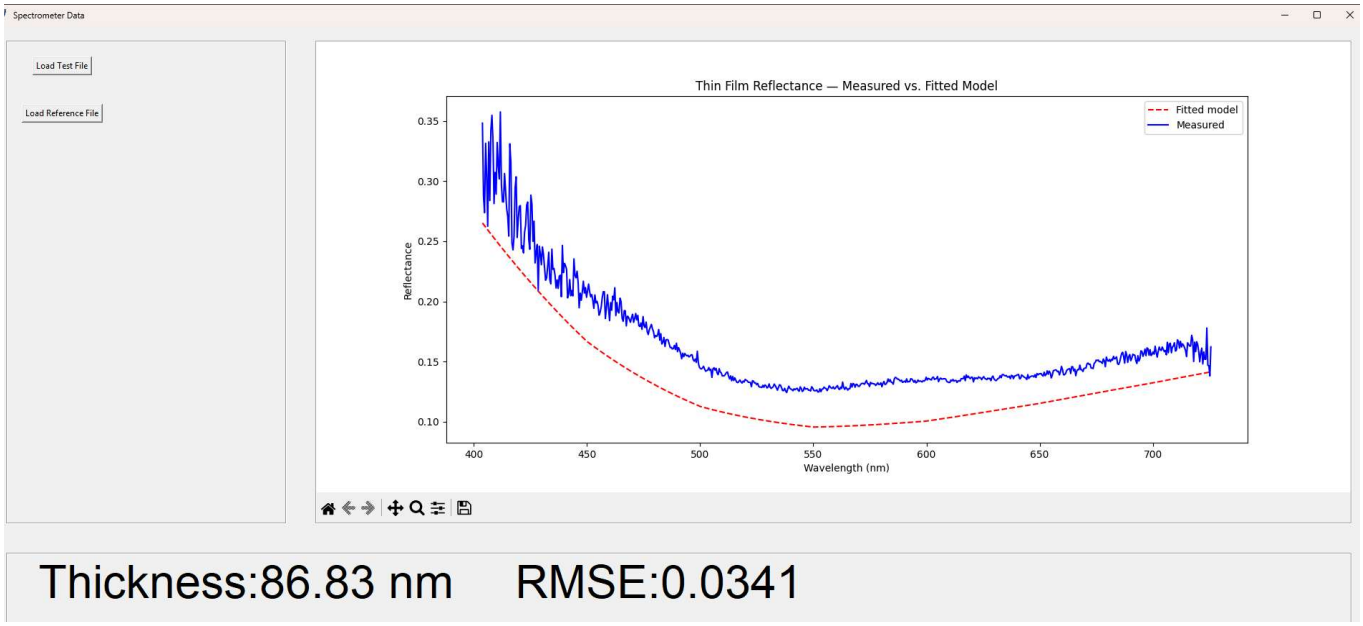
```
53    finalcalcd = optimize.minimize_scalar(cost, bounds = (1,300), method='bounded')
54    return finalcalcd
```

Bounded optimization function. Cost is a function dependent on variable d.

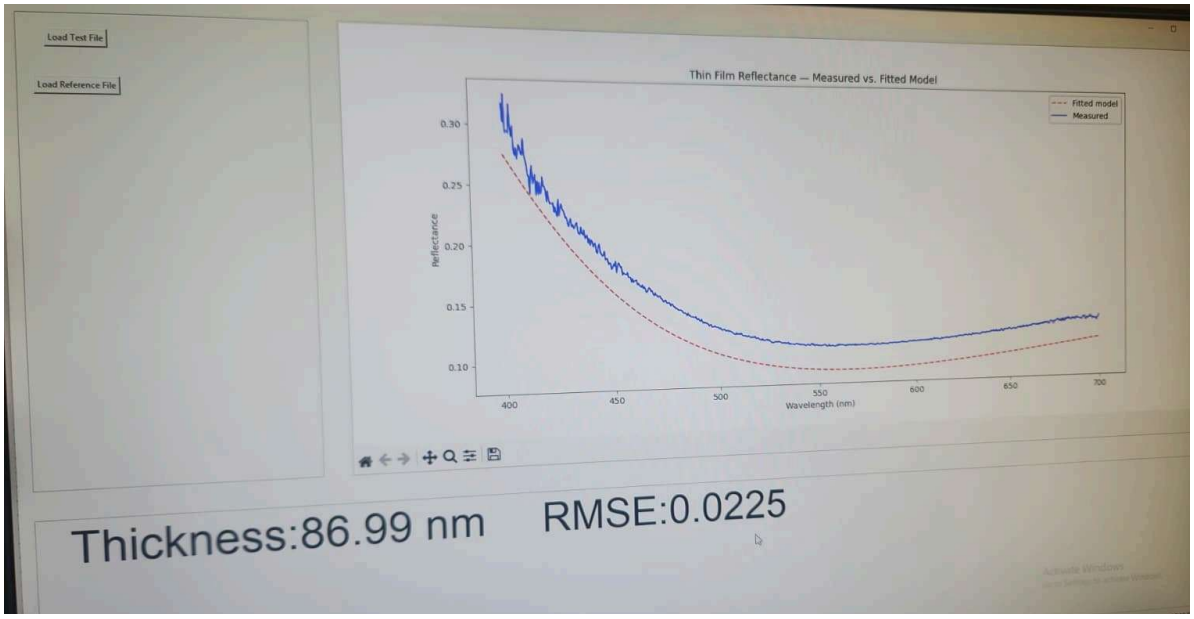
Performance

After attempting multiple trials with different wafers, we have seen successful results and expected failures. We have seen particular success with a random Silicon wafer found labeled in the lab as 100nm, with its quality of fabrication unknown. Our model found a very close curve to our intensity

measurements and produced a small Root Mean Square Error (RMSE).



These results arrived prior to taking multiple samples and averaging before utilizing the program. Ideally, there would not be drastic fluctuation in our measurements, however due to the intensity of our light requiring very small integration times (50 ms), our data is very sensitive to ambient noise. Averaging the samples before comparing against the model yielded better fit results.



Result yielded 86.99nm with an RMSE of .0225

Conclusion

While more testing is underway, the program appears promising as an unobtrusive way of measuring the thickness of the Oxide layer without introducing contaminants or physically altering the structure. Future improvements to the program will include an FFT which will allow the model to select between a vast array of Oxide thicknesses. The FFT is able to do this by distinguishing between fringes in the frequency domain. With our current model that deals with thin films this is not an issue, but in thicker films it can lead to severe miscalculations if an FFT “coarse” range is not implemented. Additionally, a model parameter selection will allow SiO_2 to be measured on other kinds of wafers such as Silver which will offer different characteristics.

One of the more interesting features of this program is that hypothetically, with a compendium of values for different material indices, we can quickly develop a model for the thickness of Silicon Oxide on any wafer. This will be prospectively tested on a wafer that has an Oxide on Silver. The results of the model will determine the feasibility of this endeavor.