COVALENT METROLOGY

COVALENT ACADEMY Q&A

Episode 14: Shining a Light on Optical Modeling for Spectral Ellipsometry

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01

Q: How does one determine the number of oscillators to use when fitting data with an oscillator-based model?

A: The short answer is to use as few as possible while still accurately modeling the measured spectra. If there are spectral regions where the model does not match the measurement well and an added oscillator will significantly improve the match, inclusion of this additional oscillator is most often justified. By contrast, if the addition of an oscillator does not improve the overall match between the model-generated and measured spectra, it is usually extraneous and should not be included. Evaluating the effect of individual oscillators on the overall MSE as well as the associated parameter error bars and correlation coefficients are the main ways that the suitability of an oscillator is determined. Consequently, the process of developing an optical model, particularly for materials where the optical properties are unknown to start, is somewhat of an iterative process that often involves some trial and error with testing various configurations and combinations of oscillators.

02

Q: Is Nanocrystalline Si the same as polycrystalline Si?

A: The category of polycrystalline Si is typically broken down into sub-categories based on average crystalline grain size. Nanocrystalline Si is a type of polycrystalline Si with the smallest grains that are generally on the order of nm in size. Since the grains themselves are so small, a non-negligible percentage of the total volume is made up of grain boundaries which, themselves, contain amorphous material. Consequently, nanocrystalline Si differs somewhat from its other, larger-grain polycrystalline Si counterparts (such as multisilicon) in that it is effectively a mixture of crystalline and amorphous phases of Si.

03

Q: Generally how does one verify or at least become comfortable with uniqueness of fit?

Becoming comfortable with the uniqueness of a model fit involves much of the same concepts as for the answer to question #1 above. There is usually a combination of conditions that the model will ideally satisfy. For instance, in an oscillator-based model, checking to see if the addition of oscillators does not substantially lower the error function and the removal of oscillators significantly increases the error function is a common strategy. Ensuring that the error bars on individual floating model parameters are low is also important (there is no universal rule, but I often prefer an error bar to be around 10% of the parameter value or less). Even further, the correlation coefficients between pairs of fit parameters is also an excellent measure of how unique a fit is since it provides quantitative information about how coupled the effects of parameters are. Ideally these will be low which indicates that there is only one set of parameter values that produces the best fit.

More broadly, checking for convergence between multiple different modeling configurations can help provide additional confidence in the accuracy and uniqueness of a result. An example of this which I described briefly later in the webinar was between modeling the optical properties of a material using an oscillator-based approach in addition to fitting for the optical properties directly from psi and delta using a direct wavelength-by-wavelength method. Finally, successfully application of a model to the measurement of multiple separate samples is also usually a good indication that the model is an accurate representation of these types of materials true properties as opposed to a coincidentally good fit for just a single sample.

04

Q: For double side polished samples, do you have issues with reflection from the polished backside? If so, how would you mitigate those effects?

A: Yes. If the detector is collecting light that is coming from reflections from the front side of the substrate and the back side of the substrate, the effects of incoherent backside reflection must be accounted for in order to accurately model the measurement. There are a few options for handling this. The best options are those that avoid collecting the backside reflection entirely. If physically roughening the backside is an option, this is the most common method. Alternatively, if ratio between substrate thickness and beam diameter is high enough, the front side and back side reflections will be spatially separated enough so that only the front side reflection can be collected by the detector aperture.

If collection of back side reflections is not avoidable, the optical model can be configured in such a way as to include the effects of backside reflections. The back side reflection model correction can fit the depolarizing effects resulting from back side reflections and therefore correct for these reflections effects on the psi and delta ellipsometric spectra.

05

Q: What is the spot size on the substrate typically?

A: This is an instrument specific detail and instruments can be configured with a wide variety of spot sizes. Our JA Woollam RC2-DI instrument has a normal beam diameter of ~5 mm. This is a typical size for most ellipsometers. Our instrument is also equipped with optional focusing optics that focus the beam diameter down to ~300 µm. One thing to keep in mind is that these numbers are the beam diameter. Since ellipsometry is most commonly measured at oblique angles of incidence, often in the range of 50 – 80º, the beam projection on the surface of the sample will be larger since the size of its interaction footprint on the sample smears out in the plane of incidence.

06

Q: Is there a limit on how thick of a layer one can measure? Can I measure a stack of thin SiN (70-100 nm) on very thick 10-20um of oxide on a silicon substrate?

A: Although there is no universal limit on the thickness of layers that can be measured and modeled, there is a decreasing accuracy in the ability to model measurements as layers get thicker and thicker. As a rule of thumb, the ideal thickness range for maximum modeling accuracy of layers that are transparent is in the range of 10-100 nm. Usually, above a thickness of about 1 µm, there will be two issues. The first is that the measured ellipsometric spectra are dominated by thin film interference oscillations (Fabry-Perot interference fringes) and even minute mismatches between the model-generated and measured spectra can introduce interference-fringe-related spectral artifacts into the optical properties of a layer. The second is that if there is any inhomogeneity present in the layer (even slight inhomogeneity), these effects are magnified as a result of the longer path length through the film and can significantly complicate the modeling.

For most practical needs, the sample you describe, thin SiN on 10-20 µm SiO_2, is not a great candidate for ellipsometry, although not necessarily impossible. At that underlying oxide thickness, there would be degraded sensitivity to the optical properties of the SiN layer its thickness. The effects of the SiN layer would certainly be well within the range of what is detectable. Don't hesitate to contact us (hello@covalentmetrology.com) if you'd like to discuss the details of potential measurements in more detail.

07

Q: Can you map out 300mm wafers? Are your tools that large?

A: Yes! The JA Woollam RC2-DI that we have installed at Covalent Metrology is configured to map substrates up to 300mm in diameter with a fully customizable scan resolution and pattern. Please contact us (hello@covalentmetrology.com) and we'd be happy to discuss details of any measurements you are interested in.

08

Q: What would be the main issues working with glass substrates vs. silicon when it comes to sensitivities of system/optical path alignment?

Working with the same system, Silicon samples do not seem to have as much sensitivities to lamp alignment/calibration of the optical path, however there seems to be a significant contribution from the alignment to the glass measurements -- what would be the root cause of those issues? And how one could control that?

A: Generally, silicon and glass substrates will both have very smooth, flat surfaces which are ideal for ellipsometry. In our experience, the overall alignment of the optical path through the system is primarily related to how smooth and flat a the surface of the sample to be measured is and therefore there is not much difference between silicon and glass (both work well). Without knowing more details about the specific issues you are referring to for alignment of a glass sample, it's challenging to identify the root of the problem. One definite difference between silicon and glass is the overall reflectance from the surface of glass is much less than that of silicon so the signal intensity at the detector will be lower. Additionally, glass is transparent over a wider spectral range so perhaps backside reflections are playing a role in alignment challenges.

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