Some Insight on Obtaining the Right Index, Extinction and Thickness Values

We'll take a look at three examples of building a model to elucidate how to build confidence that you have the correct values of the index of refraction, n, extinction coefficient, k, and film thickness as a result of your analysis of the spectroscopic ellipsometer measurements. We'll examine three measurement model fits, the Cauchy dispersion model, the Tauc-Lorentz dispersion model and the Lorentzian dispersion oscillator.

The Cauchy dispersion model is empirical. It is used for transparent materials away from the band gap and absorption bands of the material to be measured. Consider Figure 1 for SiO_2 and Al_2O_3 in the visible. The index of refraction, n, of transparent materials is usually flat at longer wavelengths, and slightly curve up as you approach shorter wavelengths due to the increased interaction between the light and molecules of the material under examination.

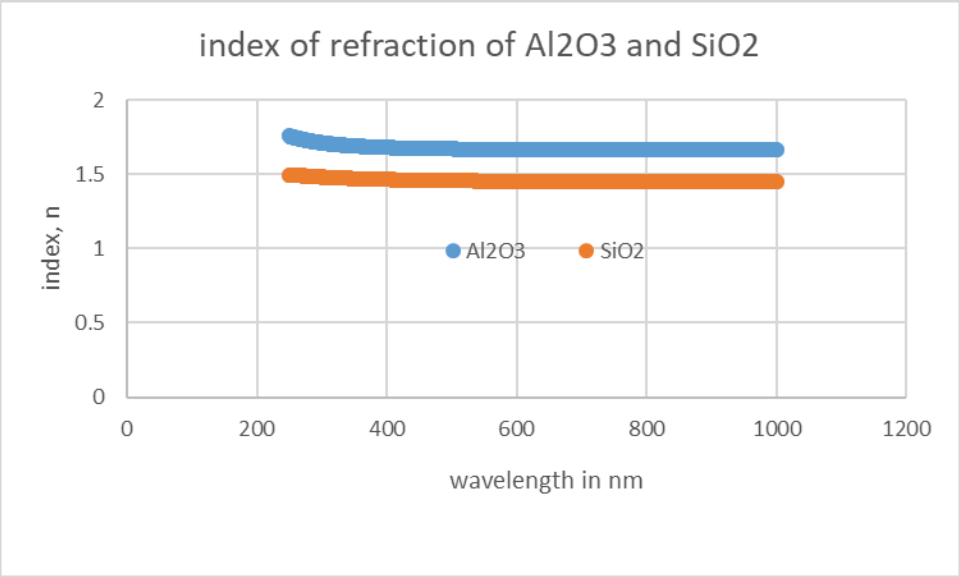

Figure 1, index of refraction for Al_2O_3 and SiO_2

To fit n, we may start with the Cauchy empirical model,

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

A is the index of refraction at long wavelengths; *B* and *C* determine the curvature of the index as λ goes to shorter wavelengths. To begin the model, you can start by looking up the index of refraction of the material and setting that number equal to *A*. Next you can pick an initial *B* based on how steep the curve is at short wavelengths. If the *A* and *B* are close enough to their real values, by iteration, you should end up with a good fit. In most cases the index fit by varying *A* and *B* will suffice. There is no need to use *C* (set *C* = 0).

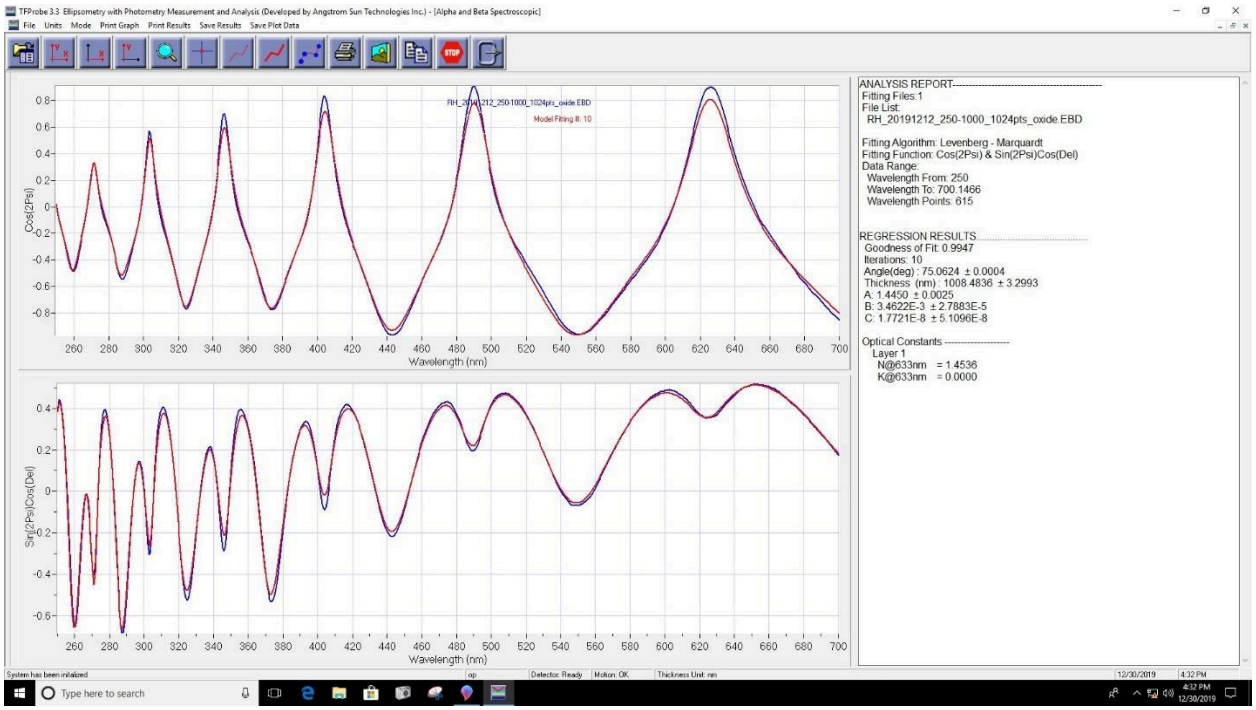

Figure 2, Ψ and Δ interference fringes for A PECVD SiO_2 film

As an example, suppose you have a PECVD SiO_2 film and you want to measure the index and thickness. We first use the tool to measure the change in the polarization state of the incident light, as described by ψ (related to the amplitude) and Δ (related to the phase), while the incident light goes through the film. As a result, you will see interference fringe oscillations caused by the light reflecting off of the cover-film and film-substrate interfaces – see Figure 2. Now that we have a measured ψ and Δ, we want to make a model using an index and thickness to match the ψ and Δ we have measured. So, next, we vary the incident light transmission/reflection coefficients as defined by the index of refraction and thickness of the film to obtain different model ψ, Δ values. We then minimize the difference between the measured ψ, Δ values and the model ψ, Δ values. When the measured ψ, Δ values are the same as the model ψ, Δ values (their difference is zero or some very small predetermined number), the index and thickness used to obtain these model ψ, Δ values must be the correct ones. It is important to fit all peaks and valleys of the fringes as we want to be sure that our iterative solution of the difference between the measured and model ψ, Δ values is at a global minimum and not a local minimum. This last point has more to do with math than physics, however, it is an important one.

As an example of a very thin film, we take a look at an atomic layer deposition Al_2O_3 film. In this case, interference fringes may not fully develop as light does not travel a long enough distance between the cover and substrate to cause the fringes to evolve – see Figure 3.

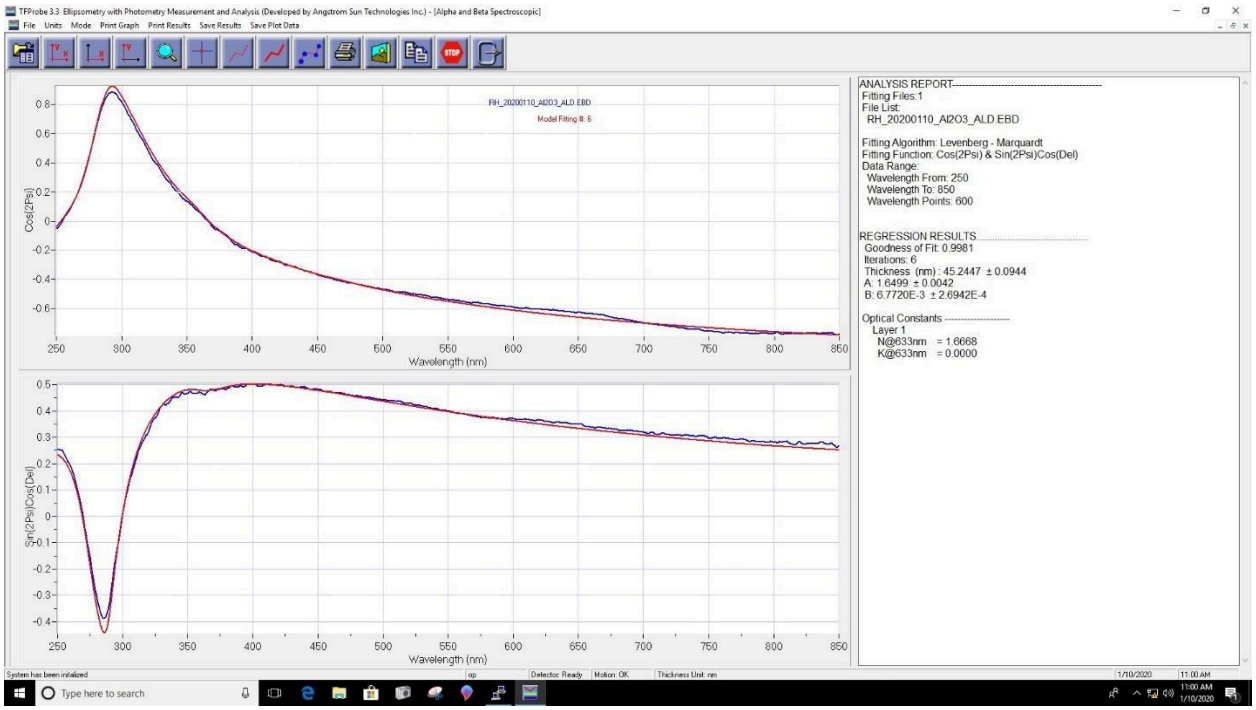

Figure 3, Ψ and Δ interference for a thin atomic layer deposition Al_2O_3 film

The Tauc-Lorentz Model

The Tauc-Lorentz model considers the imaginary part of the material's dielectric function such that it includes the bandgap of the material. Above the bandgap, there is light-material interaction. Below the bandgap, the light-material interaction is set to zero. This is a good, simple starting point for describing the optical functions of dielectrics and semiconductors. If the light is below the bandgap, it is transmitted with no interaction, if the light is above the bandgap, there will be interaction of the light with matter. So, if we use light that is a bit higher in energy than the bandgap, then we should be able to use this model to obtain reasonable Ψ and Δ results. The imaginary part of the dielectric function may be modelled by,

$$\varepsilon_i = \frac{AE_0C\left(E-E_g\right)^2}{\left(\left(E^2-E_0^2\right)^2+C^2E^2\right)} * \frac{1}{E} \quad for\ E > E_g \quad , \quad \varepsilon_i = 0\ for\ E \leq E_g$$

A, is the peak emission response for the conduction band density of states, E_0, is the position of the peak emission response, and *C*, is the width of the emission response. To obtain further insight, let's look at the equation with parameters in graph form,

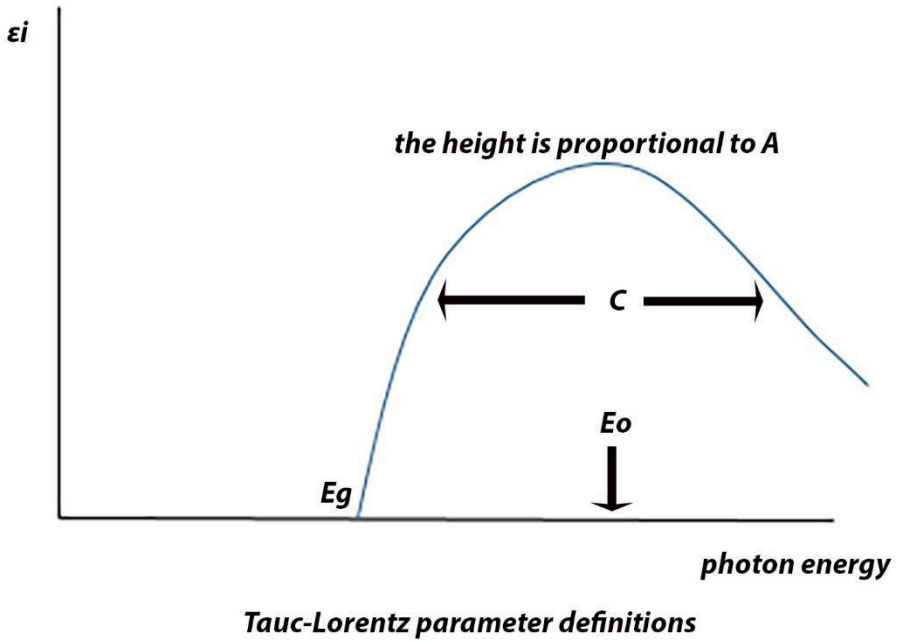

Figure 4, Tauc-Lorentz parameter definitions

Now, by looking up the different parameters of the material, if you can find them, you should have a good starting point for solutions of Ψ and Δ. At the very least, you can look up the material's bandgap, and by inspection (taking educated guesses) find reasonable values of *A*, *C* and E_0.

For example, let's consider a Si_3N_4 film deposited on a Si wafer from the Tystar 9 furnace. First, we measure the film to obtain its Ψ and Δ parameters. Next, we do a literature search about the Tauc-Lorentz model for Si_3N_4 to help with the parameters. The bandgap of crystalline Si_3N_4 is approximately 5.0 eV [1]. From the same reference, E_0 ~ 10 eV and C ~ 10 eV. These are good starting points for our model. The peak emission response will depend on how the film was deposited – percent amorphous, number of contaminants, etc., so, we'll have to take an educated guess on this one. From the graph of the same reference, let's start out with a response of about 200. So, just using these numbers, we get a model Ψ and Δ map, and compare them to their measured values, as shown in Figure 5.

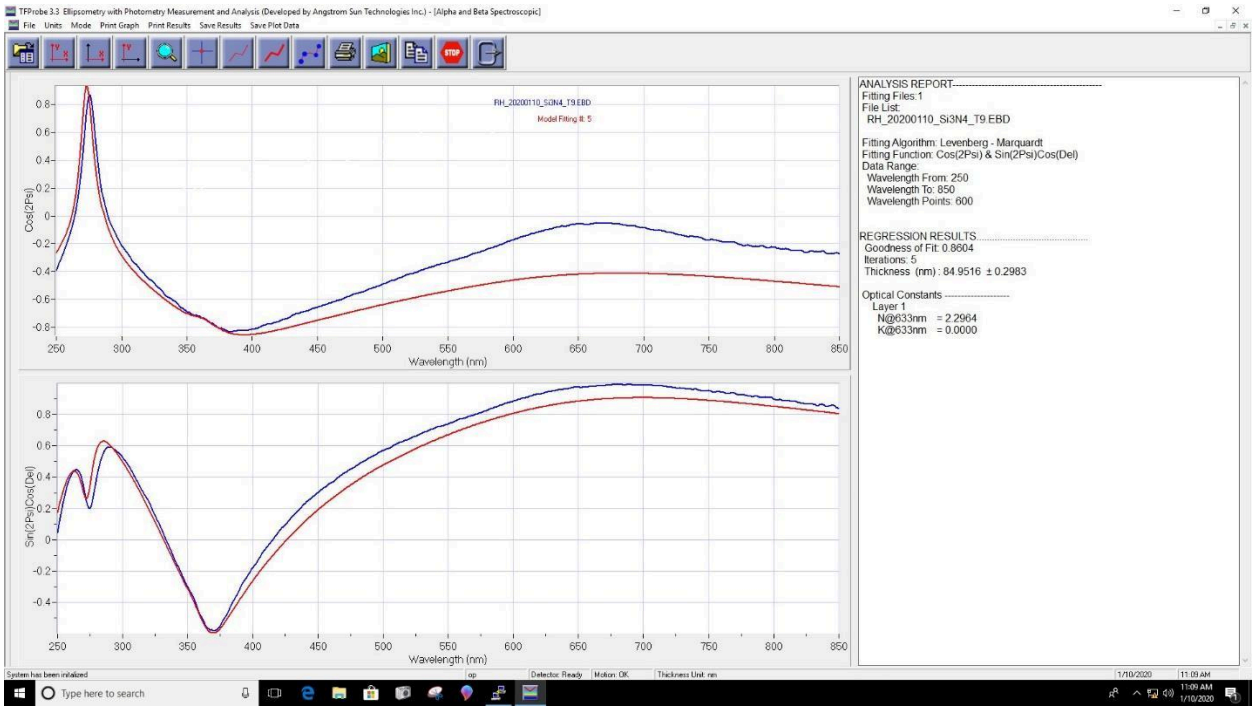

Figure 5, Ψ and Δ with initial nitride model parameters

This first result is not so bad. The model Ψ and Δ generally follow their measured values. Now, we let *A*, *C*, E_0 and E_g vary to get a better fit. The result is shown in Figure 6.

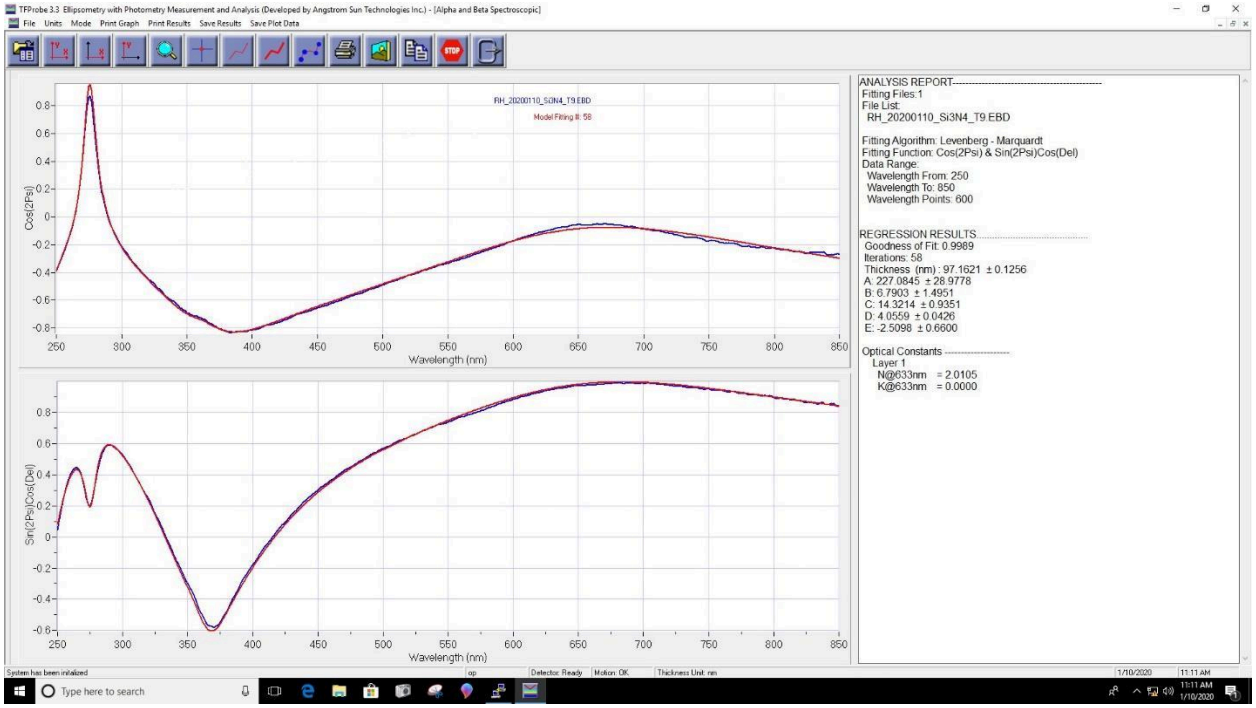

Figure 6, Ψ and Δ with fitted nitride model parameters

Lorentz Absorption

Sometimes with our measured Ψ and Δ, we encounter local peaks in the graph caused by enhanced material response to the incident light. For instance, In the measured values for Si_3N_4 there is a mild peak around 650nm where the model and the measured values of Ψ and Δ differ a bit. We don't expect a large change in the resultant values for n, k and film thickness, but it would be useful to see if we can fit the curve more accurately. We note that the peak is not infinite in extent, and does not have more than one local extremum. We'd like to add another oscillator model to the original one to take into account this local response. The Lorentzian line is a standard response of a molecular system to incoming light. It has three main parameters which can define the structure of the response – how intense the response is, *A*, at what central wavelength the response happens, λ_0, and how broad is the response, γ. The Lorentzian oscillator may be modelled by,

$$\varepsilon_r = \frac{A\lambda^2\left(\lambda^2-\lambda_0^2\right)}{\left[\left(\lambda^2-\lambda_0^2\right)^2+\gamma^2\lambda^2\right]} \quad , \quad \varepsilon_i = \frac{A\lambda^3\gamma}{\left[\left(\lambda^2-\lambda_0^2\right)^2+\gamma^2\lambda^2\right]}$$

where, ε_r, is the real part of the dielectric function, ε_i, is the imaginary part of the dielectric function, and λ is the wavelength.

Suppose, as an example, we'd like our fit of the previous Tauc-Lorentz model of Si_3N_4 to include the mild peak located near 650nm. We'll do the same as we did before. Start with an initial, reasonable guess and then let the software, through iteration get us a better answer. Okay – we figure λ_0 is 650nm, but what about γ and *A*? We'll measure the width of the peak near 650nm, γ, and set it equal to 100nm. For the response, *A*, we'll just go in increments of 0.01, 0.1, 1.0 etc. Until we get some movement of the model's peak towards its respective measured value. In fact, let's just let the software iterate all three values for optimization. Table 1 compares the Tauc-Lorentz and Tauc-Lorentz+Lorentz oscillator results. Figure 7 shows the Tauc-Lorentz + Lorentz oscillator Ψ and Δ graph.

	Fit	**n @ 633nm**	**k**	**Film thickness nm**
Tauc-Lorentz	0.9989	2.01	0.00	97
Tauc-Lorentz + Lorentz oscillator	0.9990	2.02	0.00	96

Table 1, Comparison of results from the two models for Si_3N_4

As we predicted there are no major changes, but it does give some indication of how the fit changes, and how the n, k and film thickness will change in this particular instance. One can continue to add Lorentzian oscillators to take care of all local peaks that are not accounted for by the original Tauc-Lorentz model. There seems to be two more, one at 750nm and one at 850nm. The same procedure would be used to further fit the curve. However, for the purposes of our demonstration, the present values of n, k and film thickness will suffice.

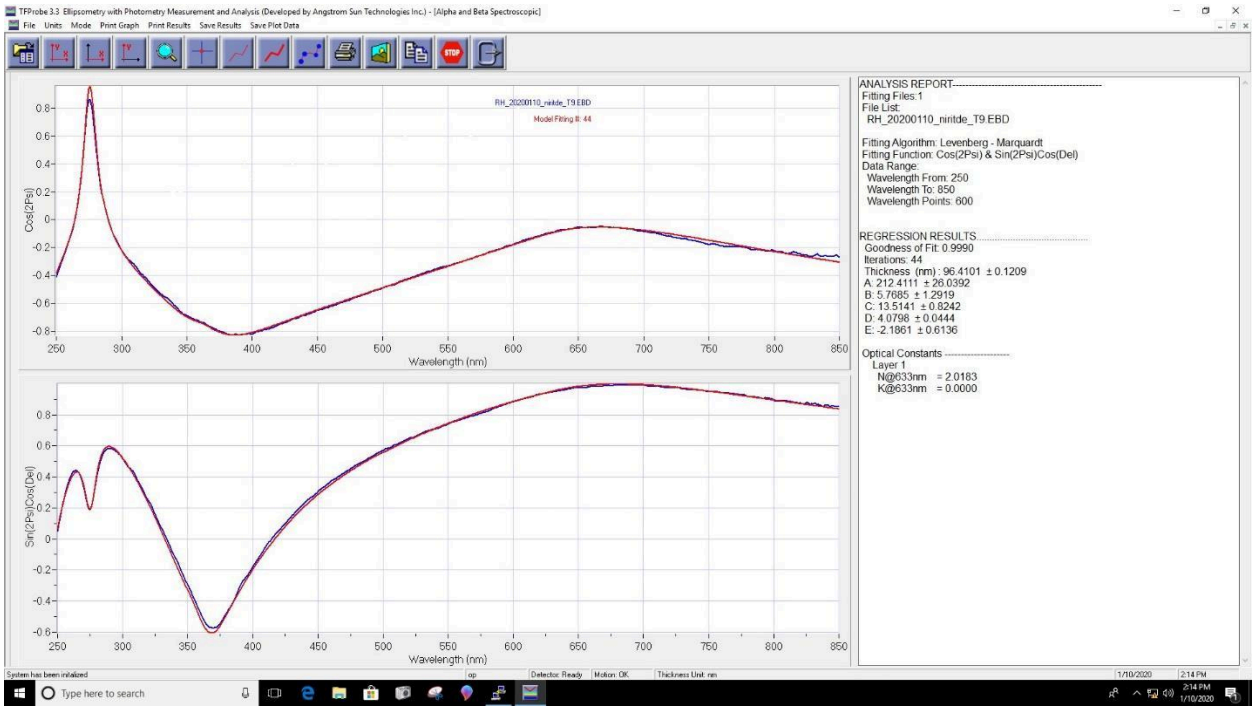

Figure 7, Si_3N_4 Tauc-Lorentz model including one Lorentz oscillator centered at 650nm

Caveat-Emptor – when fitting the Lorentz oscillator model it is important to take into account all of the factors that create the peak. In the above case, we have two sources that produce the interrogating light, a deuterium lamp and a halogen lamp. The deuterium lamp has a strong peak around 650nm (Figure 8), so the gentle peak in the Ψ and Δ map is probably due to the enhanced brightness of the source. In fact, this is the case, so there is no physical response from the film at 650nm. The source gives the peak near this wavelength. The important point here is that one has to take into account not only the response of the film, but the spectrum of the source to make sure you obtain the correct fit. As a result, in this case, we'll stick with the Tauc-Lorentz model alone for the values of n, k and the film thickness.

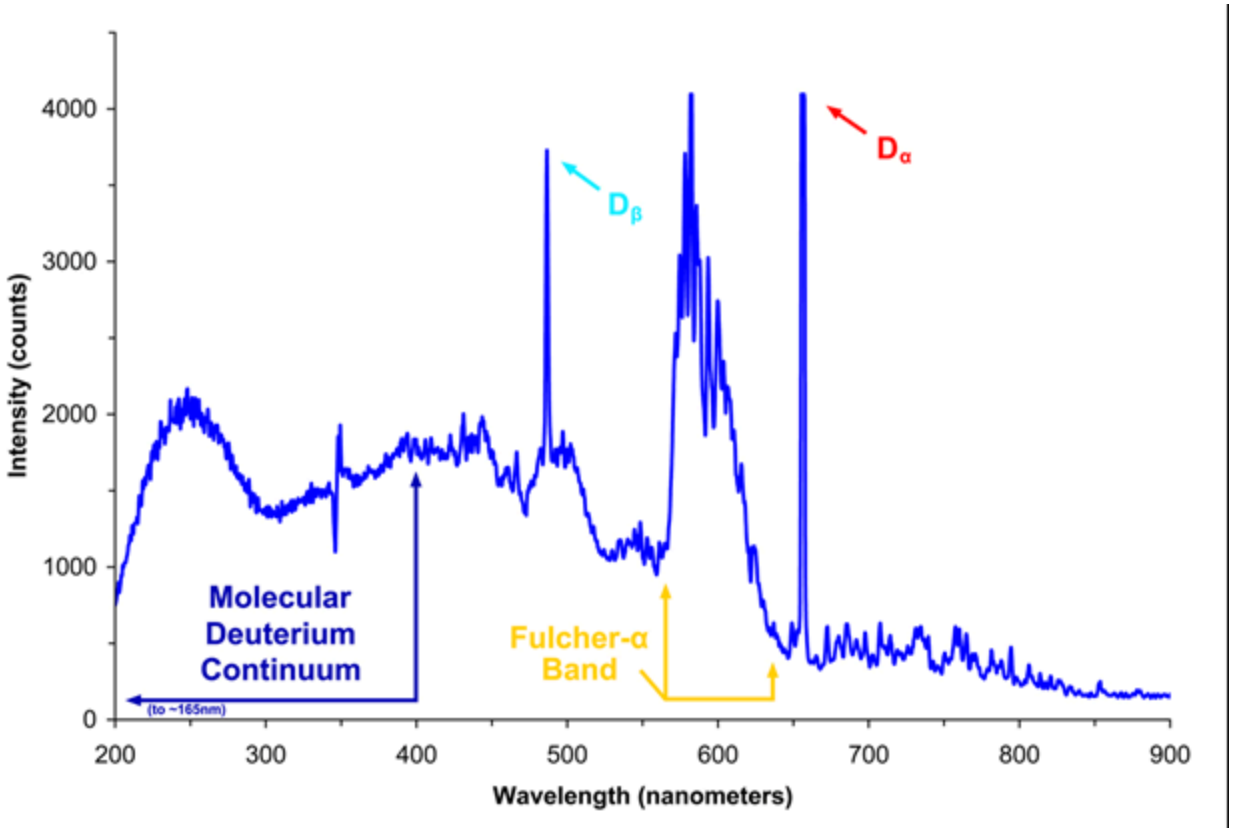

Figure 8, spectrum of the deuterium source

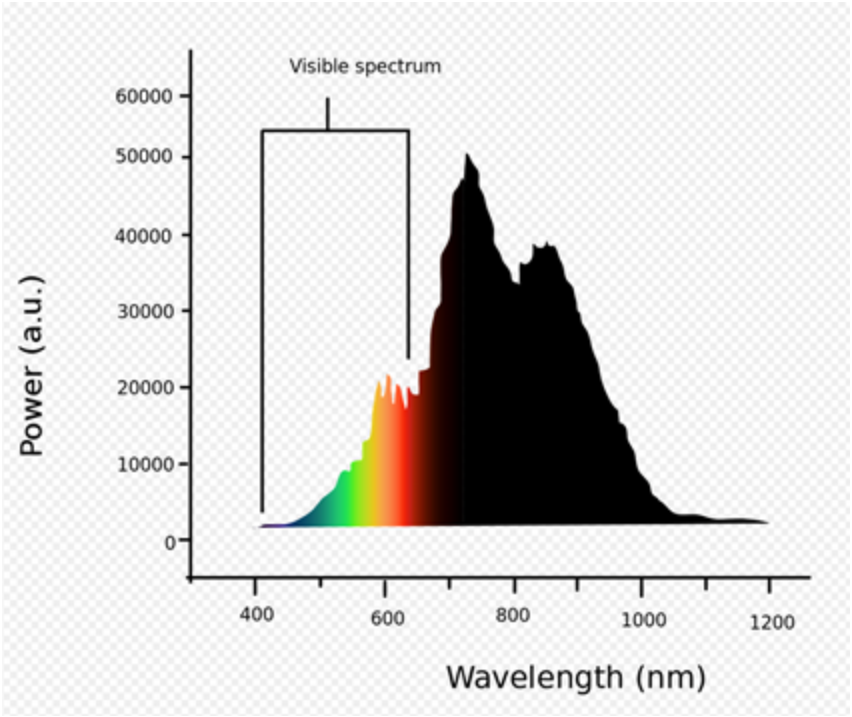

Figure 9, spectrum of the halogen source

[1] Gritsenko, V. A., “Electronic structure of silicon nitride”, Uspekhi Fizicheskikih Nauk, Russian Academy of Sciences, 55 (5) 498 – 507 (2012)