Case study II: Modelling the transmission of a thin film

Ivan Biaggio
Department of Physics, Lehigh University, Bethlehem, PA 18015, USA
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This is our second “case study”: The data set is a measurement of the transmission of a thin film on a glass substrate as a function of the wavelength. Can we extract both the thickness of the film and its refractive index dispersion?

This time our data is the transmission of a thin film of some unknown material on top of a glass substrate. The data has been measured for three films of different thickness.

Through appropriate curve fitting, we want to extract information on

1. The refractive index of the thin film material and its wavelength dependence. Assume that the refractive index of the substrate is 1.5.

2. The thickness of the material.

3. The absorption of the material. Assume that the absorption of the substrate is just 0.

For the refractive index of the material, try modeling it again with a Sellmeier Formula [1] of the kind

$$n(\lambda)^2 - 1 = \frac{S_1}{1-(\lambda_1/\lambda)^2}, \tag{1}$$

where S_1 and λ_1 represent the strength and the position of the oscillator. Now, this form may or may not be appropriate for fitting the thin film transmission data. You actually have four options: (0) Use a constant value for the refractive index; (1) use Eq. (1) as is; (2) add another oscillator, as we did earlier; or (3) just add a constant to the right-hand side of Eq. (1), because a constant would be the limit for an oscillator that is very far away at short wavelengths. The advantage option (3) has over option (2) is that you have one less parameter. But you can try to experiment to see if there is something to gain with the additional parameter. In addition, you should try first to fit with options (0) and (1), which are simpler. Even if they don't give you a good fit they allow you to get an idea about what is going on and if the rest of the procedure is working well.

Next, you need to assume something for the absorption of the film. You need to do this because the transmission drops to zero below 650 nm. The simplest method is to use a single absorption line, with a certain strength and width, and described by a Gaussian function. Hence;

$$\alpha(\nu) = \alpha_0 e^{[-(\nu-\nu_0)/\Delta\nu]^2} \tag{2}$$

with $\nu = c/\lambda$. Note that this is a function of frequency. There are physical reason for assuming that the resonance energy of something can be broadened in a Gaussian way. It would make no phyiscal sense to assume a Gaussian in wavelength like $\exp([(\lambda-\lambda_0)/\Delta\lambda]^2)$.

Finally, in order to fit the spectra you need to develop a formula for the transmission of the sample as a function of wavelength, thickness, absorption, and refractive index. As a hint, here is the *amplitude* transmission coefficient (minus some phase factor) of a thin film of thickness d that has an absorption α sitting on a substrate, when the light is incident upon the film:

$$t_f = \frac{t_{af}t_{fs}}{1-r_{fa}r_{fs}e^{2idk}e^{-\alpha d}}e^{-\alpha d/2}, \tag{3}$$

where the coefficients t_{fs}, r_{fs} are the normal incidence Fresnel transmission and reflection coefficients, respectively, for the amplitude of the wave when it passes from

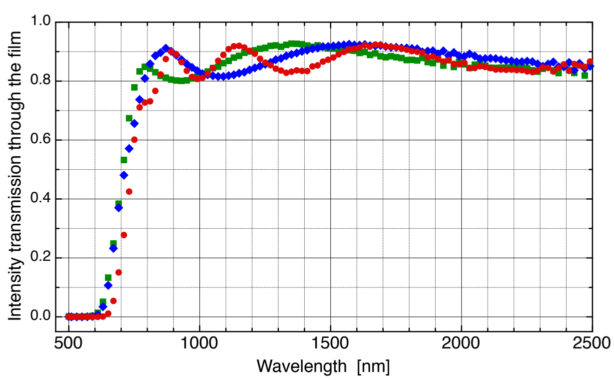

FIG. 1. Data for the transmission spectrum of three thin films consisting of the same material

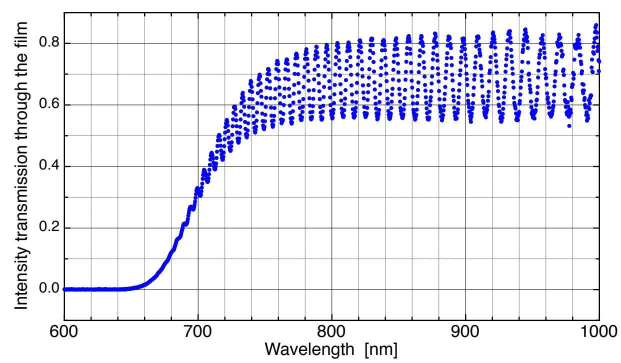

FIG. 2. Data for the transmission spectrum of another film, consisting of a different material.

film to substrate, from air to film (af), film to air (fa), and so on. But note that Eq. (3) gives the *complex* transmission coefficient for the *amplitude* of the wave. You need to write the full expression for the *power* transmission of the film/substrate assembly, which will depend on the absolute value squared of t_f, and will also include a loss factor $(1 - R)$ for the reflection loss at the interface between substrate and air.

Assignments

Investigate this problem. Determine both the refractive index dispersion and the thickness of the films. Discuss what issues need to be taken into account, and how you addressed them.

At the end, also look at the second data set, in Fig. 2, and discuss what are the issues when fitting that particular data set.

Write a short report. Make 10 copies or so that you distribute at our next meeting, so that everyone has a copy of what everyone else did.

Philosophical note

I have seen people rely on literature to solve this problem, one example being Ref. 2. I am opposed to such a procedure because it is so much more cumbersome and complicated (just look at all the formulas in Ref. 2 as compared to all the formulas in what I wrote above), much slower, and less precise than the straightforward curve fitting procedure described above.

The curve fitting, done right, is faster, simpler, and delivers the information that you need in a cleaner way.

Basically, the philosophy is always to fit the results of an experiment with a complete mathematical model that is able to predict the outcome of the experiment from the physical parameters that you need to measure. More old-fashioned things like extracting information from particular features of the data (contrast ratio, peak positions) are good as a sanity check, but are not necessarily good as the only way of determining physical parameters.

[1] W. Sellmeier, "Zur Erklärung der abnormen Farbenfolge im Spectrum einiger Substanzen," Annalen der Physik und Chemie **219**, 272-282 (1871).

[2] R. Swanepoel, "Determination of the thickness and optical constants of amorphous silicon," J. Phys. E: Sci. Instrum. **16**, 1214 (1983).