

Characterisation of Multilayer Thin Films on the Aquila nkd



This application note demonstrates the principle of analysing multilayer thin films on the Aquila nkd Spectrophotometer.

One of the main advantages of the nkd spectrophotometer is its ability to analyse not just single films and substrates but multiple layers of thin films and coatings. Such layer systems are often devices in themselves and the thickness of each layer is critical in their operation. For the purposes of this illustration we will examine a polymer substrate coated with four alternating layers of high quality refractory oxides SiO_2 and Ti_2O_3 .



Figure 1. Schematic of sample

The substratematerial is unknown and Ti_2O_3 is a material which can exhibit considerable variability in its optical constants. It will be necessary to investigate these differences along with the layer thicknesses. The measurements were made using unpolarised light at 30 degrees incidence.

To begin analysing an unknown material, three steps are required. First, advanced analysis mode is selected and then the analysis method - Powell, LM or Global. LM is modified version of the Levenberg-Marquardt method. It is the fastest regression technique, and is best suited when starting the fitting from an approximate solution. Powell is a slower method than LM, but is more robust. It is typically used to refine a solution once the starting values have been found. The Global analysis method is based on the Simplex method and will generally find the right answer given time.

Next the dispersion model is chosen for each layer and finally the initial parameters of the model for each layer. The Cauchy model can be used to describe transparent materials such as BK7, ITO, SiO_2 , MgF_2 , etc. The Drude-Lorentz model can be used with dielectrics, semiconductors and metals.

The choice of starting values for the model parameters in Drude-Lorentz and Nanoptix is crucial. Some experimentation may be required to find reasonable starting points for new materials.

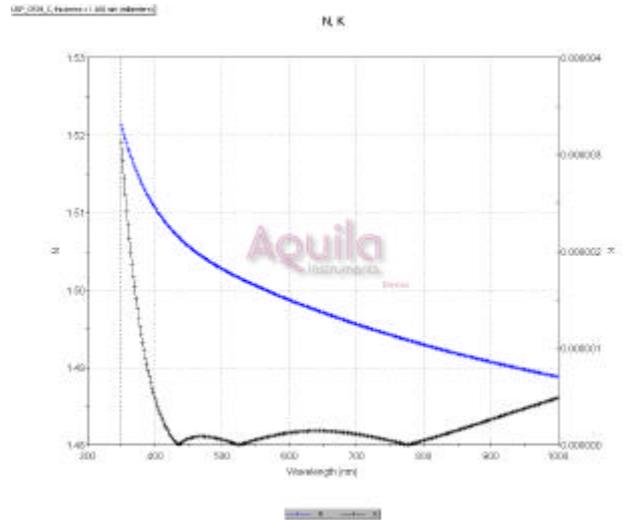


Figure 3. n & k for substrate

The raw T and R data for the substrate is presented in Figure 2. An initial analysis was performed using the Cauchy model which adequately describes simple transparent materials such as this, which do not exhibit highly structured T and R spectra. The absorption is very low throughout the visible region (450-750nm) and rises very sharply below 400nm. The small bumps in the k spectrum throughout the visible are artefacts of the fitting procedure. In reality k is flat and very close to zero. The numbers are so small that they are unlikely to affect analysis of the subsequent layers.

The next step is to analyse the substrate plus the first layer. Figure 4. below is the T and R measurements for the substrate plus one layer of Ti_2O_3 . The characteristics of the substrate were entered from the material database and Pro-Optix™ was asked to calculate n, k and d of the Ti_2O_3 layer only. In performing the analysis, if the first pass does not give a good fit, it can be necessary to pick a new starting thickness, reset the initial parameters and try again. The model parameters are adjusted and finally a coherence factor was added. The final fit for the substrate plus one layer of Ti_2O_3 can be seen on this expanded plot. A value of 34.2nm for the layer has been deduced and the n & k values are plotted in Figure 5. This layer is then added to the materials database.

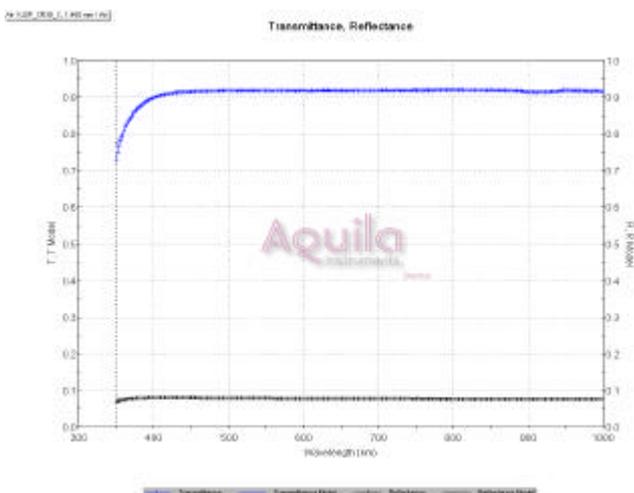


Figure 2. Substrate T & R measured and fitted

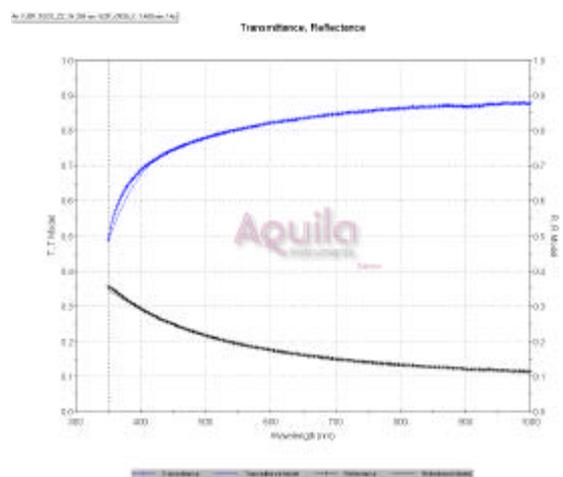


Figure 4. Substrate T & R measured and fitted

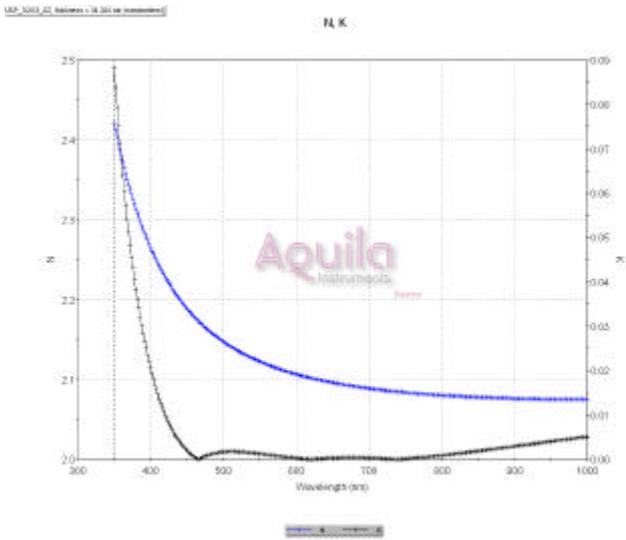


Figure 5. n&k for the first layer – Ti₂O₃

The next step is to measure a sample with two layers, Ti₂O₃ and SiO₂. Figure 6 below, is a plot of this measurement and the resulting fit, achieved by entering the two known materials, the substrate and Ti₂O₃ layer, into the analysis and asking Pro-Optix™ to calculate n, k and thickness of the SiO₂ layer only. The SiO₂ layer was found to be 28.4nm thick and the resulting n & k curves are shown in Figure 7. Having characterised the Silica layer, this is then entered into the database also, as a new material.

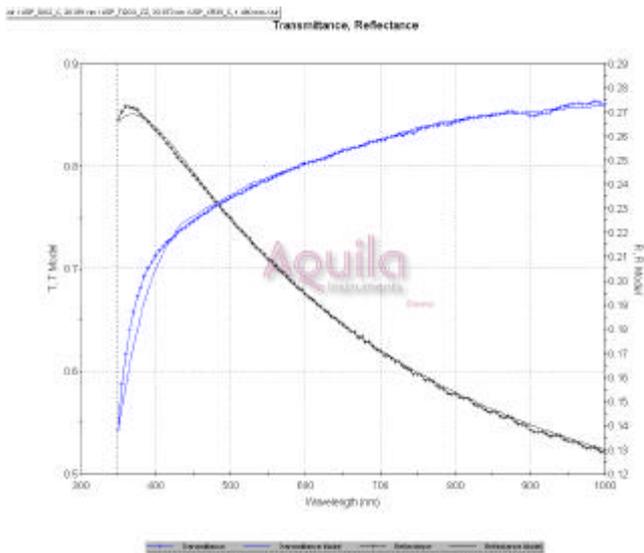


Figure 6. Substrate + 2 layers T & R measured and fitted

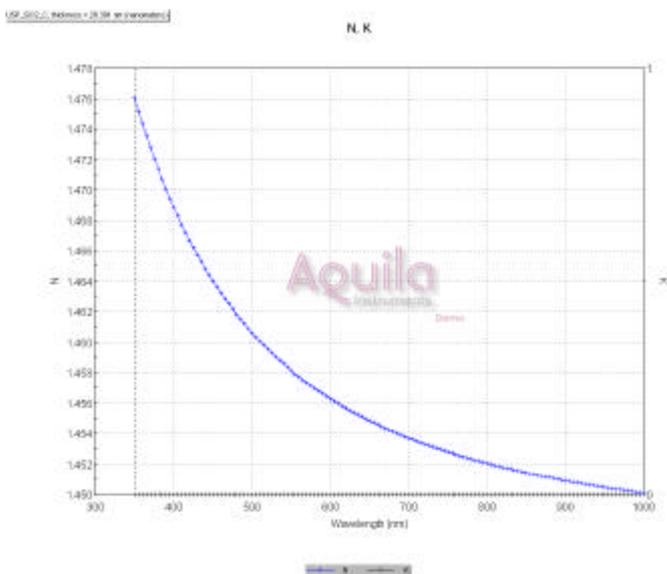


Figure 7. n & k for second layer – SiO₂

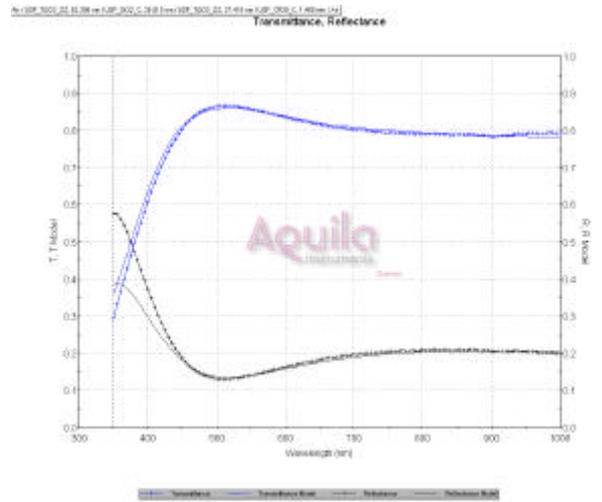


Figure 8. T & R measured and fitted for substrate + 3

The three materials are now known to Pro-Optix™, greatly simplifying subsequent analysis of the multilayer system. For the next sample of the substrate plus three layers, the materials are simply input from the database and only the thickness of the various layers is allowed to vary. Figure 8 is the T and R plot for this system of layers and the resulting layer thicknesses are shown in Figure 9, exactly as they are presented in Pro-Optix™.

File:	USP_T003_T
Thick:	62.147 nm (nanometers)
Find n:	Yes Find d: Yes
File:	USP_S002_C
Thick:	27.380 nm (nanometers)
Find n:	No Find d: No
File:	USP_T003_C
Thick:	34.140 nm (nanometers)
Find n:	No Find d: No
Substrate:	USP_CR38_C
Thick:	1.400 nm (nanometers)
Find n:	No Find d: No

Figure 9. Layers thicknesses for substrate + 3 layers

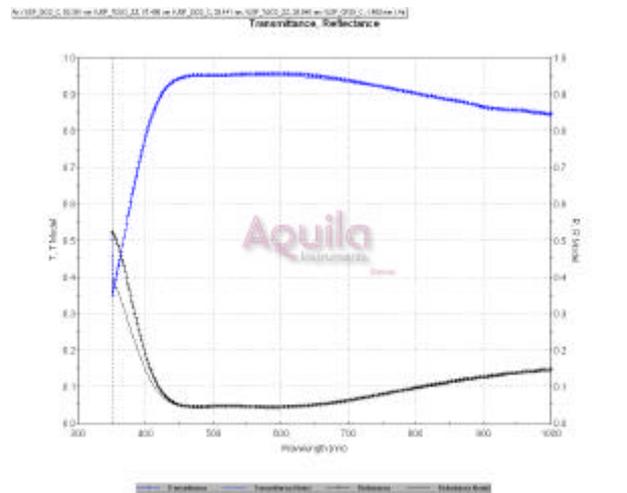


Figure 10. T & R measured and fitted for 4 layers

File:	USP_S002_C
Thick:	93.381 nm (nanometers)
Find n:	Yes Find d: Yes
File:	USP_T003_ZZ
Thick:	57.438 nm (nanometers)
Find n:	No Find d: No
File:	USP_S002_C
Thick:	35.441 nm (nanometers)
Find n:	No Find d: No
File:	USP_T003_ZZ
Thick:	26.948 nm (nanometers)
Find n:	Yes Find d: Yes
Substrate:	USP_CR38_C
Thick:	1.400 nm (nanometers)
Find n:	No Find d: No

For four layers, the same technique is used and the results for this are shown in Figures 10 and 11.

It can be seen then that the nkd spectrophotometer, along with Pro-Optix™ provide a precise and comprehensive method of characterising thin multilayer films and substrates. A system of layers of known or new materials, can be analysed and defined with just a few simple steps. The nkd spectrophotometer has been designed specifically for this purpose and offers an accurate and elegant approach to an otherwise complex measurement.

Figure 11. Layers thicknesses for substrate + 4 layers