

Characterisation of TiO₂ Thin Films and Multilayer Antireflective Coatings by Spectroscopic Ellipsometry

Céline Eybert - Application Scientist - Thin Film Division

TiO₂ films are extensively studied because of their interesting chemical, electrical and optical properties.

TiO₂ is a high bandgap semiconductor that is transparent to visible light and has excellent optical transmittance. TiO₂ has high refractive index and good insulating properties, and as a result it is widely used as protective layer for very large scale integrated (VLSI) circuits and for manufacture of optical elements. Additionally TiO₂ films have potential uses for a number of electronic device applications such as dye-sensitized photovoltaic cells as well as antireflective (AR) coatings, gas sensors, electrochromic displays, and planar waveguides. The high dielectric constant of TiO₂ allows its consideration as an alternative to silicon dioxide for ultrathin gate oxide dielectrics used in memory and logic devices. Several methods have been used to prepare titania films, and these include chemical vapour deposition (CVD), pulsed laser deposition, reactive sputtering and sol-gel deposition. The sol-gel technique has emerged as one of the most promising techniques as this method produces samples with good homogeneity at low cost.

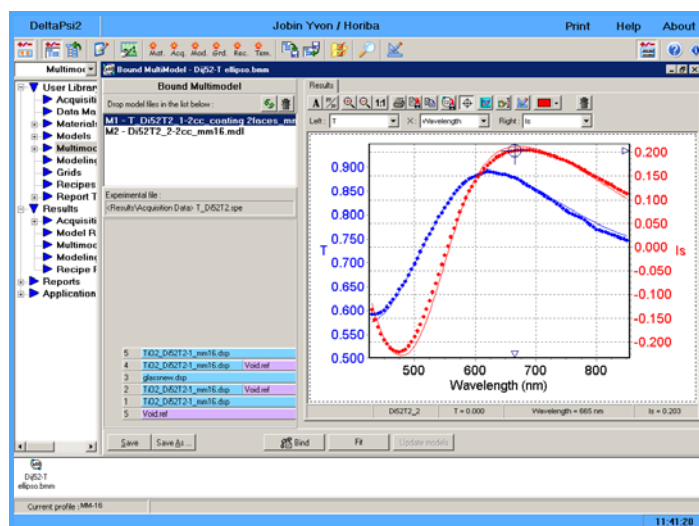
To achieve optimum performance it is important to characterise the optical constants and thicknesses of thin TiO₂ layers accurately.

In this note, we show how the Spectroscopic Ellipsometry (SE), non-destructive optical technique is particularly suitable for thin film characterisation.

Characterisation of TiO₂ Thin Films

For this work TiO₂ films were prepared by dip coating on the pre-treated glass substrate. This technique allows to deposit the AR coatings on both sides of the glass substrate.

The work was performed using a HORIBA Jobin Yvon MM-16 Spectroscopic Ellipsometer, with an automatic goniometer. To achieve this characterisation both reflection and transmission ellipsometry were performed. Ellipsometric measurements were collected at an angle of incidence of 70° across the spectral range 430-850 nm, with spectroscopic transmission data acquired at normal incidence. HORIBA Jobin Yvon DP2 software allows the measurement and use of multiple data types, and the simultaneous analysis of these two models was achieved by the **Bound Multimodel** function. From the simultaneous analysis of all data, both refractive index and film thicknesses were obtained without ambiguity.



The New Amorphous dispersion formula was used to model the refractive index for TiO₂.

$$n = n_{\infty} + \frac{B_i (\omega - \omega_i) + C_i}{(\omega - \omega_i)^2 + \Gamma_i^2}$$

$$k(\omega > \omega_g) = \frac{f_i (\omega - \omega_g)^2}{(\omega - \omega_i)^2 + \Gamma_i^2} \quad k(\omega \leq \omega_g) = 0$$

$$B_i = \frac{f_i}{\Gamma_i} [\Gamma_i^2 - (\omega_i - \omega_g)^2] \quad C_i = 2 f_i \Gamma_i (\omega_i - \omega_g)$$

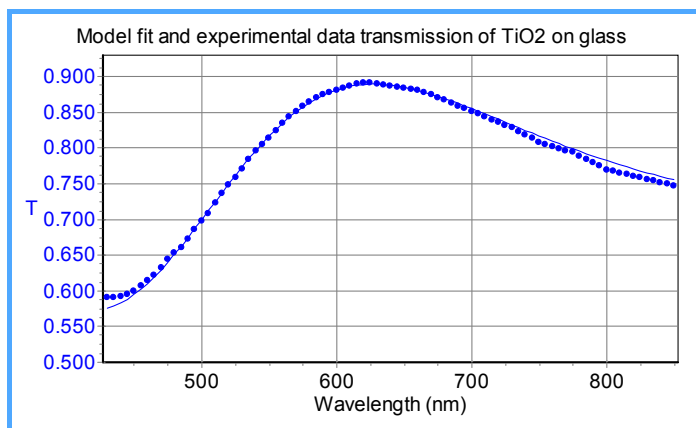
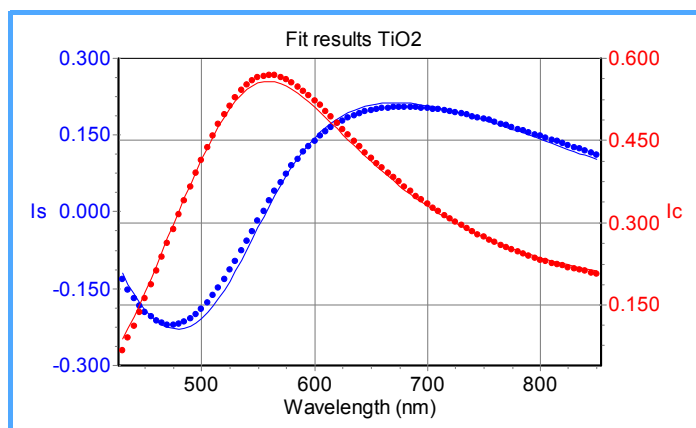
The New Amorphous dispersion formula is a rewriting of original Forouhi-Bloomer formula (Phys. Rev.B, 34, 7018 (1986)).

The best model comprises of two layers with the bottom layer being less dense than the top layer, and takes into account the AR coatings deposited on the both sides of the glass substrate.

The DP2 Software includes advanced features for the automatic correction of backside reflections from transparent substrates.

TiO ₂	776Å
93% TiO ₂ /7% void	796Å
Glass substrate	
93% TiO ₂ /7% void	796Å
TiO ₂	776Å

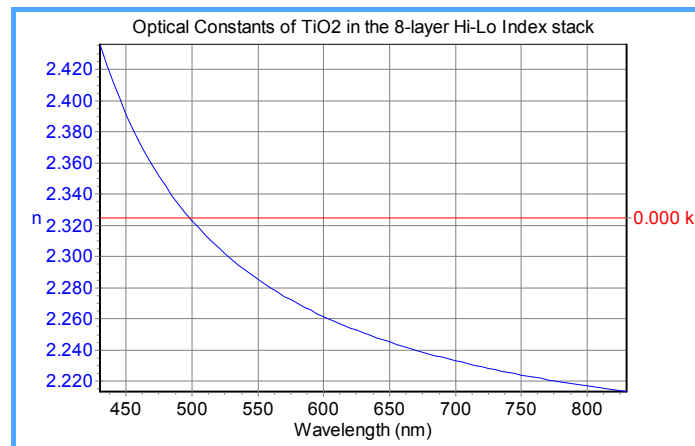
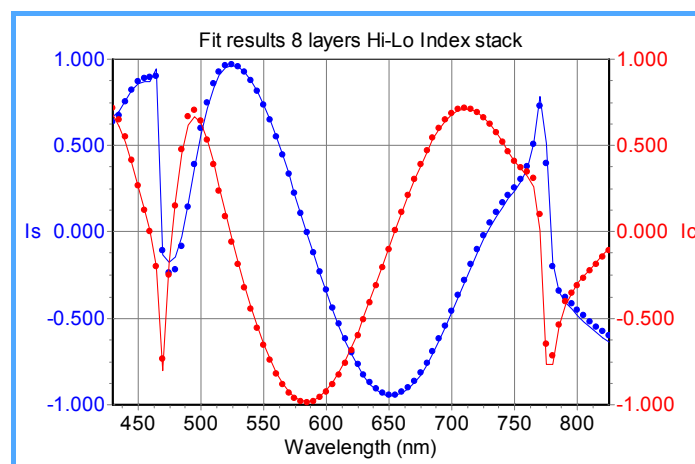
TiO ₂
SiO ₂
TiO ₂
SiO ₂
Si substrate



Characterisation of TiO₂ in 8-layer Hi-Lo Index Stack

The analysis was performed with the MM-16 Spectroscopic Ellipsometer across the range 430-830 nm at an incident angle of 70°.

The best fit model was obtained using a 8-layer model. DP2 software allows characterisation of these structures using the special **Periodic Structure** and **Correlated Layer** functions that allow modelling of repeating pairs of layers used in MQW or Bragg Reflector structures.



Conclusion

Owing to the sensitivity of the MM-16 Spectroscopic Ellipsometer and the advanced modeling features included in the DP2 software, this note describes the successful characterisation of complicated anti-reflective structures. Accurate and simultaneous determination of thickness and optical properties have been performed in the visible range. Similar analyses have been applied to other high-k material such as Ta₂O₅ / glass, Al₂O₃ / 3*{A₂O₃/a-Si} / GaAs, SiO₂ / 2*{HfO₂ / SiO₂} / glass.