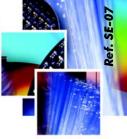
Spectroscopic Ellipsometry

Characterisation of TiO₂ Thin Films and Multilayer Antireflective Coatings



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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.

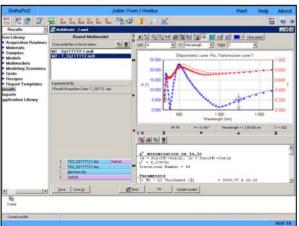
To achieve optimum performance it is important to characterise the optical constants and thicknesses of thin TiO₂ layers accurately. In this note, we show how the Spectroscopic Ellipsometry (SE), non-destructive optical technique is particularly suitable for thin film characterisation.

Characterisation of TiO₂ Thin Films

For this work TiO₂ films were prepared using a sol-gel technique, by spin coating on a pre-treated glass substrate (CNRS-LIMHP - Université Paris 13).

The work was performed using a Jobin Yvon UVISEL NIR Spectroscopic Phase Modulated 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 310-1700 nm, with spectroscopic transmission data acquired at normal incidence. Jobin Yvon DeltaPsi2 (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. The New Amorphous dispersion formula was used to model the refractive index for TiO₂. From the simultaneous analysis of all data, both refractive index and film thicknesses were obtained without ambiguity.

Bound Multimodel window of DeltaPsi2 software



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

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

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

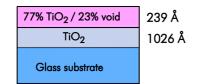
$$B_i = \frac{f_i}{\Gamma_i} [\Gamma_i^2 - (\omega_i - \omega_g)^2] \qquad C_i = 2 f_i \Gamma_i (\omega_i - \omega_g)$$



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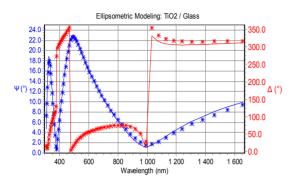


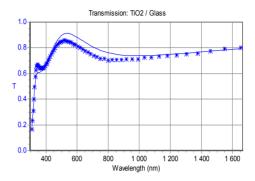


TiO2 Optical Constants

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2,800
2,700
2,600
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The best model comprises of two layers with the top layer being less dense than the bottom layer. The top layer is calculated by the addition of void using the Effective Medium Approximation.

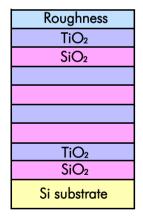


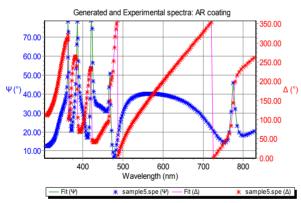


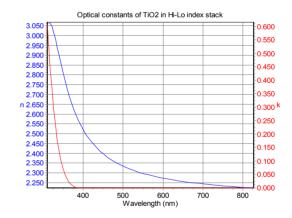
This work was performed in collaboration with Lamia Znaidi from the CNRS - LIMHP - Université Paris 13

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

The analysis was performed with the UVISEL Visible Ellipsometer across the range 310-830 nm at an incident angle of 70°. The best fit model was obtained using a nine-layer model that included a roughness layer at the sample surface. 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

The characterisation of TiO_2 as a single layer and as an 8-layer dielectric stack was successfully carried out with the UVISEL Spectroscopic Phase Modulated Ellipsometer. Accurate and simultaneous determination of thickness and optical properties have been performed in the NIR/Visible range. Similar analyses have been applied to other high-k material such as Ta_2O_5 / glass, Al_2O_3 / $3*{A_2O_3/a-Si}$ / CaAs, CaAs

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