Characterization of SiO_2 on glass by Spectroscopic Ellipsometry

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Abstract

It is always a challenge for spectroscopic ellipsometry to characterize transparent films on transparent substrates, not only due to the low index contrast between materials but also due to the backside reflection from the substrate.
This application note emphasizes the sensitivity of the UVISEL phase-modulated spectroscopic ellipsometer by presenting its abilities to characterize two different samples of SiO_2 layers on glass substrate.
The key point for such applications is to measure with high accuracy the low values of parameter Δ and its variations over the full spectral range and to take into account backside reflection from the glass substrate.

Key words

Spectroscopic Ellipsometry, transparent films on transparent substrates, optical properties, low index contrast, backside reflection

Introduction

The chemical compound silicon dioxide, also known as silica, is an oxide of silicon with the chemical formula SiO2. It has been known for its hardness since ancient times. Silica is most commonly found in nature as sand or quartz, as well as in the cell walls of diatoms.

Silica is manufactured in several forms including fused quartz, crystalline, pyrogenic silica (or fumed silica), colloidal silica, silica gel, and aerogel. Silica is used primarily in the production of glass for windows, glassware, and beverage bottles, but also finds many other uses. The majority of optical fibers for telecommunications are also made from silica. It is a primary raw material for many white ware ceramics such as stoneware, earthenware, porcelain.

Silica is a common additive in the production of foods, where it is used primarily as a flow agent in powdered foods, or to absorb water in hygroscopic applications. It is the primary component of diatomaceous earth which has many uses ranging from filtration to insect control. It is also the primary component of rice husk ash which is used, for example, in filtration and cement manufacturing.

Thin films of silica grown on silicon wafers via thermal oxidation methods is very widely used in microelectronics, where they act as electric insulators with high chemical stability and as a passivation layer. It protects the silicon, stores charge, blocks current, and even acts as a controlled pathway to limit current flow.

For increased efficiency of solar cells, the silica undercoat is applied as an anti-reflection layer. This increases the amount of light transmitted to the cell, thereby increasing efficiency.

Experiment

The excellent sensitivity of the UVISEL Phase Modulated Spectroscopic Ellipsometer was demonstrated by studying of two samples of SiO2 on glass. The closeness of the refraction indices of silicon dioxide and glass is the main difficulty of this task. Both samples and the pure glass slide have been measured with a high degree of accuracy. Measurements were performed by the UVISEL at an incidence angle of 60° and 70° over a spectral range of 245 nm to 2100 nm (i.e: 0.6 eV to 5 eV).

In many cases measurements with less sensitive systems require the bottom surface of the sample to be roughened to eliminate the back surface reflection, as this otherwise distorts the signal measured
Two samples were measured without removing their backside reflections with dedicated sample preparation. The UVISEL is able to measure these samples without damaging or modifying the sample.

Figure 1: UVISEL 2

The DeltaPsi2 software features a “backside reflection model” allowing the optical treatment of the backside reflections collected during the measurement.

For the user, there is no sample preparation, and operations are performed automatically by the software.

First Example

Glass substrate

First, the pure glass substrate sample was examined. A model with thin roughness layers on both front and back, surfaces of glass have been used. Glass optical constants were determined and then used to build a model for the sample under study.

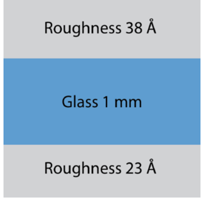


Figure 2

The fit curves and glass optical constants are given in Figures 3 and 4.

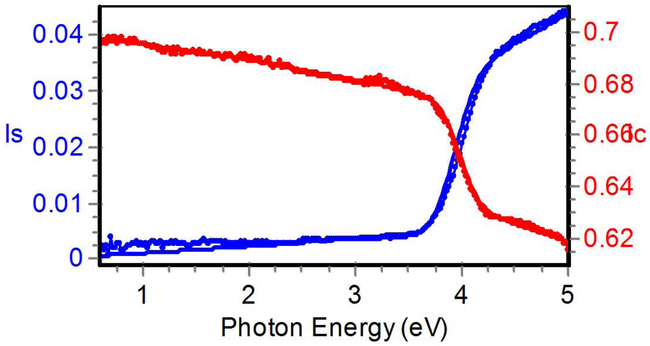


Figure 3

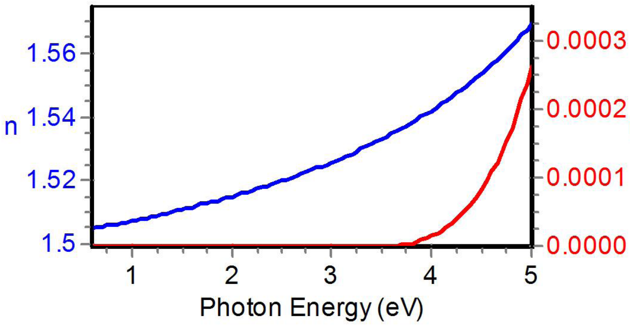
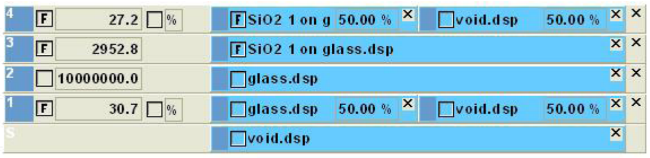


Figure 4

300 nm SiO_2/Glass

The following model, a 5 layer model (figure 5), has been used to fit perfectly the experimental data. The introduction of the SiO_2 roughness overlayer and the roughness of the backside of glass, described by the Effective Medium Approximation (50% SiO_2 + 50% void; 50% glass +50% void, respectively), has allowed significant improvements to how good the fit is, described by χ^2 value. $\chi^2 = 0.24$



4	F	27.2	☐ %	F SiO2 1 on g	50.00 %	☐ void.dsp 50.00 %
3	F	2952.8		F SiO2 1 on glass.dsp		
2	☐	10000000.0		☐ glass.dsp		
1	F	30.7	☐ %	☐ glass.dsp	50.00 %	☐ void.dsp 50.00 %
S				☐ void.dsp		

Figure 5

A film thickness of 2980 Å was found for the SiO_2 layer.

Figure 6 shows a good fit agreement between the collected data (dots) and the calculated data (solid line).

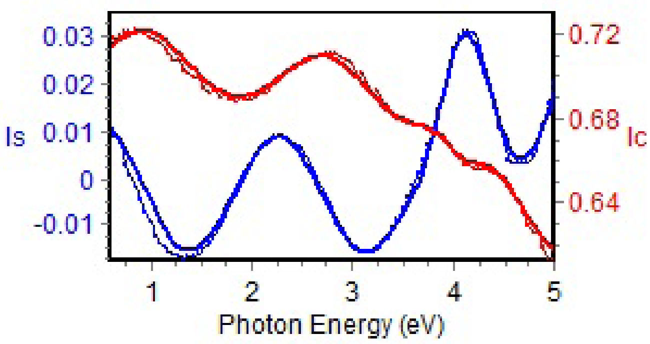


Figure 6

The spectra above shows interference fringes with small amplitude. The amplitude of the fringes is directly correlated to the low contrast index between the film and the substrate, as expected.

On Figure 7, the corresponding (Ψ,Δ) parameters are shown over the range $\Psi \in [0,90°]$ and $\Delta \in [0,360°]$. To have a better understanding of the importance of measuring the parameter Δ close to 0° , we have represented Δ over the range [-180°, 180°] on Figure 8. On this graph, we can see low variations of Δ between -2° and 3° which have to be measured with high sensitivity to be able to model such a stack.

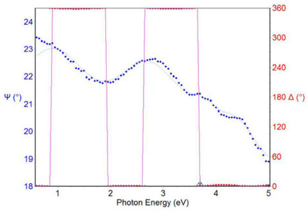


Figure 7

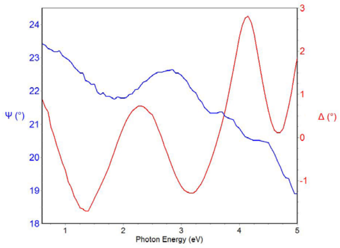


Figure 8

The optical constants of the SiO_2 layer were extracted by using a Lorentz oscillator dispersion formula and are displayed on Figure 9.

$$\varepsilon = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\omega_t^2}{\omega_t^2 - \omega^2 + i\Gamma_0\,\omega}$$

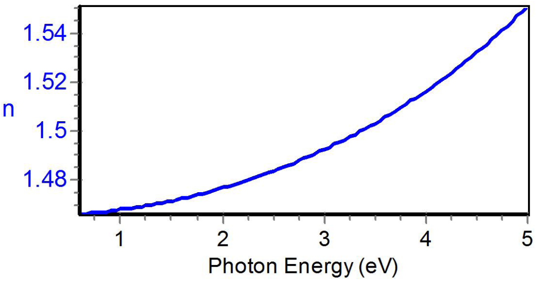
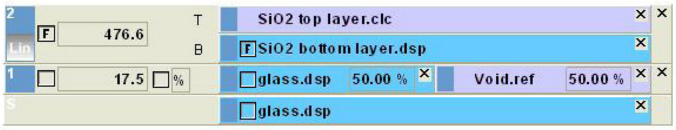


Figure 9

Second example

The model used to describe this second sample is a variation of refractive index in depth, with an index increasing with depth. This variation is described using a linear gradient. This model does not take into account the backside reflection due to thick glass substrate, which allows for geometrical separation of the beams reflected from top and bottom surfaces, respectively.



2 Lin	F 476.6	T	SiO2 top layer.clc	
		B	F SiO2 bottom layer.dsp	
1	☐ 17.5 ☐ %		☐ glass.dsp 50.00 %	Void.ref 50.00 %
S			☐ glass.dsp	

Figure 10

The thickness obtained for the SiO2 layer was 477 Å.
Figure 11 shows the raw data (dots) along with the calculated data (solid line)

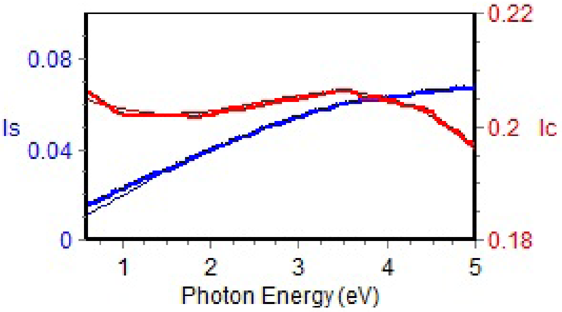


Figure 11

The SiO_2 layer refractive index shows gradient behavior, changing from a higher index at the bottom to a lower refractive index at the top. The figure below illustrates well the closeness of refractive indexes of glass and SiO_2.

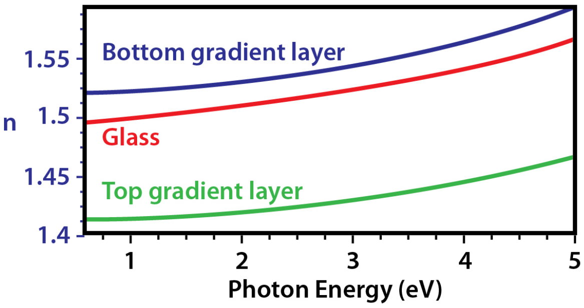
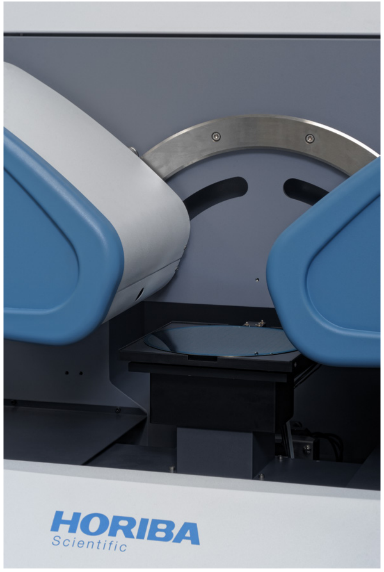


Figure 12

Conclusions

This work shows that the UVISEL Phase Modulated Spectroscopic Ellipsometer is a very sensitive instrument and is able to accurately determine both the thickness and refractive index of a SiO2 layer on a glass substrate without damaging the sample. The software is able to include not only the effects of the backside reflection, but also cases where the refractive index of the oxide is inhomogeneous with depth.

The UVISEL has been shown to be able to characterize samples with layers having refractive indices close to indices of the substrates, which is traditionally a challenging application for the ellipsometry.



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