



*Thin Film Measurement solutions  
Measurement probes, software, custom  
development and integration*

### Spectroscopic Reflectance for thin film measurement

Spectroscopic reflectance is a powerful non-destructive method of thin-film measurement. MProbe thin-film measurement system [1] is specially optimized to achieve exceptional precision and analysis capabilities. Thicknesses and optical constants of the wide range of filmstacks can be measured quickly and easily.

There are several common misconceptions about spectroscopic reflectance capabilities as applied to thin-film measurement. It is assumed, for example, that using this technique one can only determine thicknesses (one needs to know optical constants), that it has lower precision as compared with ellipsometry and that only one or two thicknesses can be determined simultaneously. These misconceptions reflect the traditional/historical use of this technique and, indeed, the capabilities of majority of commercially available instruments. However, these are not limitations of the technique but the way it is used and the data is interpreted (i.e. software analysis).

Both spectroscopic reflectometry and ellipsometry are indirect measurement methods i.e. one needs to create a model of the measured filmstack and physical parameters (thicknesses and optical constants) are inferred from the best fit of the model to the measured data. Both techniques analyze interaction of the light with the filmstack using the same Fresnel equations. Ellipsometry takes into account light's polarization and uses phase difference ( $\Delta$ ) between p and s polarization of reflected light, while spectroscopic reflectance does not use the phase difference.  $\Delta$  parameter has high-sensitivity to very thin films but this sensitivity decreases for the thicker films. In practice, spectroscopic ellipsometry has a clear advantage over spectroscopic reflectometry in following cases:

- ✓ Measurement of the very thin films <5nm
- ✓ Simultaneous measurement of T,n in case of non-absorbing films (k=0)
- ✓ Determination of the n,k values by direct inversion of measured data (special case, mostly for substrates of unknown material)

But spectroscopic reflectance has clear advantage in:

- ✓ Higher precision of thickness measurement (with exception of very thin films). MProbe precision <0.01nm
- ✓ Measurement of thick films (>10um). MProbe up to 500um
- ✓ Higher measurement speed MProbe <1ms
- ✓ Measurement of surface roughness.

Both techniques can measure complex multilayer filmstacks and can determine thickness and n,k values of the materials.

Traditionally, spectroscopic reflectance is used or assumed to be appropriate for simple thickness measurement: one or two layer filmstacks. Following are few examples

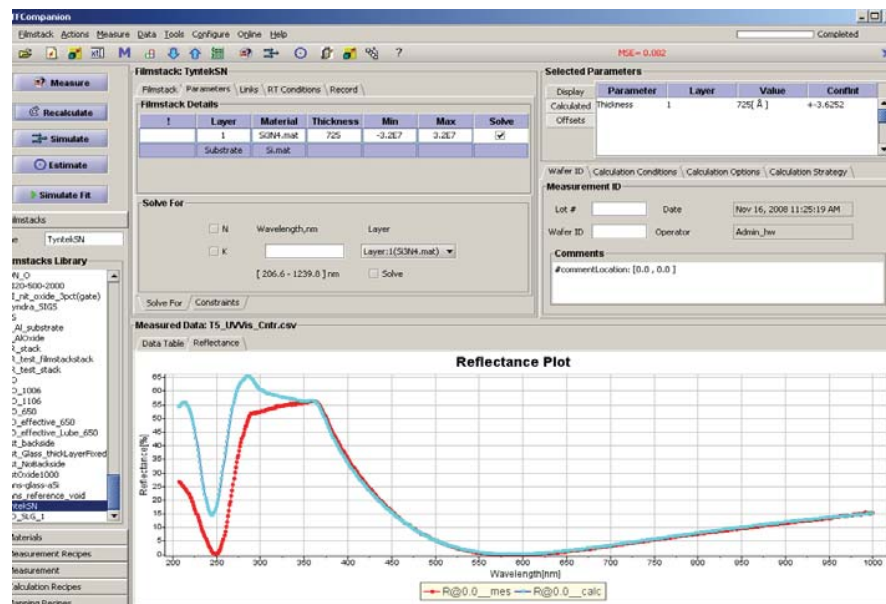
of the use of spectroscopic reflectometry that demonstrate its ability in more complex applications. Historically, measurement of the poly-Si and Si<sub>x</sub>N (Si-rich Nitride) were two major applications that brought about a widespread use of spectroscopic ellipsometry in semiconductor industry – spectroscopic reflectometry, used in traditional way, simply could not measure these applications. For this reason, it is instructive to show that spectroscopic reflectometry can, in fact, measure them very successfully – if used properly.

### Example 1. Measurement of SiN

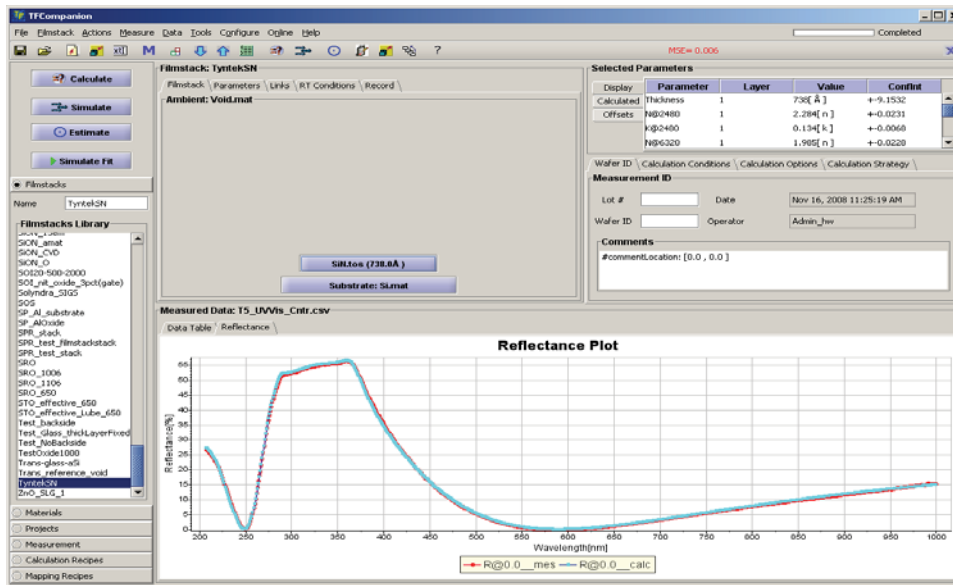
SiN is dielectric (non-absorbing) in the visible spectral range, so one can determine only thickness using reflectance measurement. Traditional approach is to measure thickness assuming known (tabular) values of the optical constants and using only visible spectrum. However, SiN is frequently non-stoichiometric and has optical constants that deviate from expected values. This approach can give a wrong thickness result, while showing reasonably good fit of the measured vs. model data. Typically, the suggested remedy is to use spectroscopic ellipsometry to determine T,n which solves the problem. However, spectral reflectance can be successfully used in this case if one notice and use the fact that SiN has absorption in the UV part of the spectrum.

Following example shows results of 700A nitride measurement in 200-1000nm range. The data was analyzed using two different approaches:

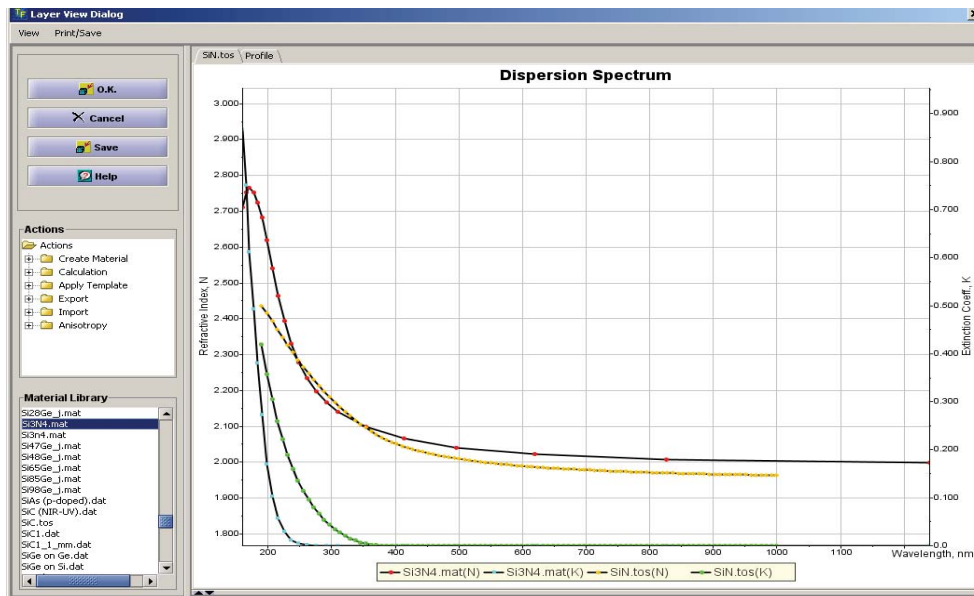
1. Use standard Si<sub>3</sub>N<sub>4</sub> material data and calculate only thickness.(only T case). (Measured thickness: 725A)
2. Represent nitride dispersion using Tauc-Lorentz approximation and determine T, n, k simultaneously (T,n,k case). (Measured thickness: 738A)



**Fig. 1 Case 1 SiN results (only T calculated).** Red is measured, blue modeled. There is a very good fit in the visible range, but discrepancy in UV shows that there is a problem



**Fig 2. Case 2 SiN results ( T,n,k calculated ). Red is measured, blue modeled. Nitride optical dispersion is represented using Tauc-Lorentz approximation**



**Fig. 3 Comparison of SiN standard (stoichiometric) and measured optical constants dispersion. Measured k shows earlier onset of absorption that is indicative of Si-rich nitride.**

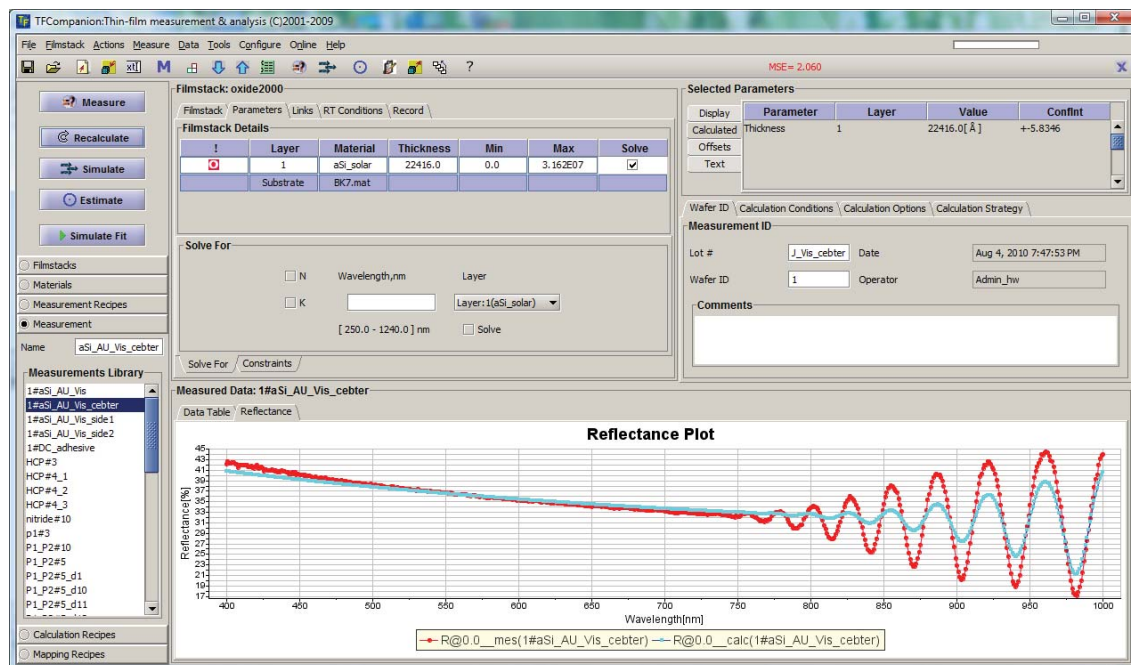
## Example 2. Measurement of polycrystalline/amorphous Si.

Polycrystalline Si used widely in many applications from semiconductor chips to solar cells. For this example, aSi was deposited on a glass substrate and annealed (crystallized) with a goal to use it as an absorber of the solar cell. The layer thickness was estimated  $\sim 2 \mu\text{m}$ . The measurements were taken in 400-1100nm range. Thick aSi layer was completely opaque in 400-740nm range, so only 740-1100nm range was useful for analysis.

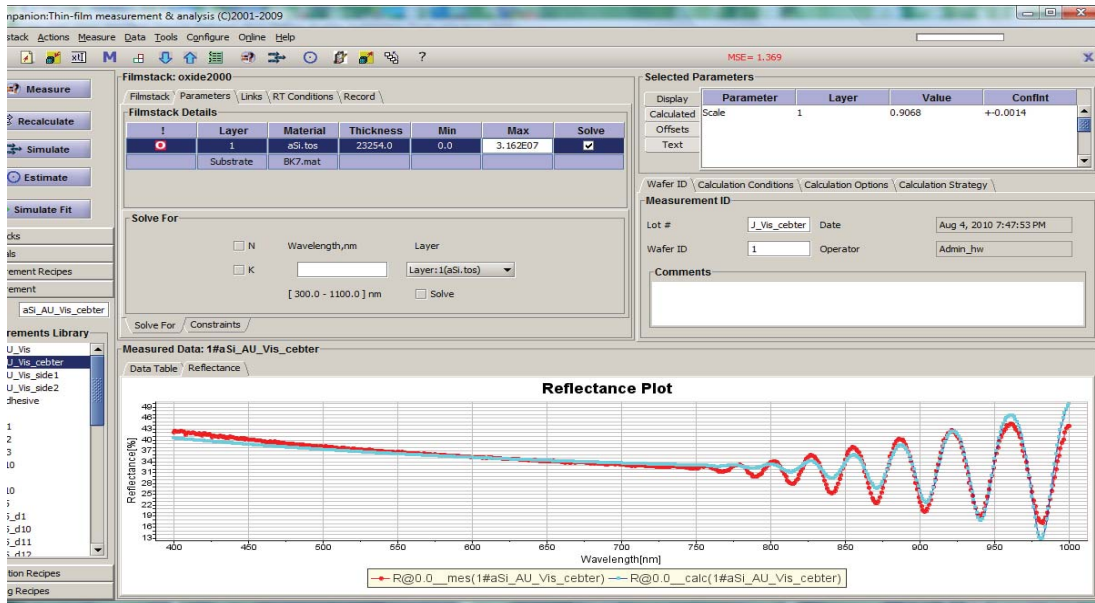
Spectral reflectance measurements were analyzed using two approaches:

**Case 1 (Traditional approach):** Similar sample was measured using spectroscopic ellipsometer to determine optical constants. These optical constants were used in analysis of the data i.e only T was extracted. Results are shown on Fig. 4. The fit of the model to measured data is not very good but reasonable

**Case 2:** Use Tauc-Lorentz dispersion approximation to model optical constants of poly/aSi and determine T,n,k values simultaneously.



**Fig. 4 Case 1(traditional approach).** Measurement only T of poly-Si.  
Determined thickness is 2.24 $\mu\text{m}$



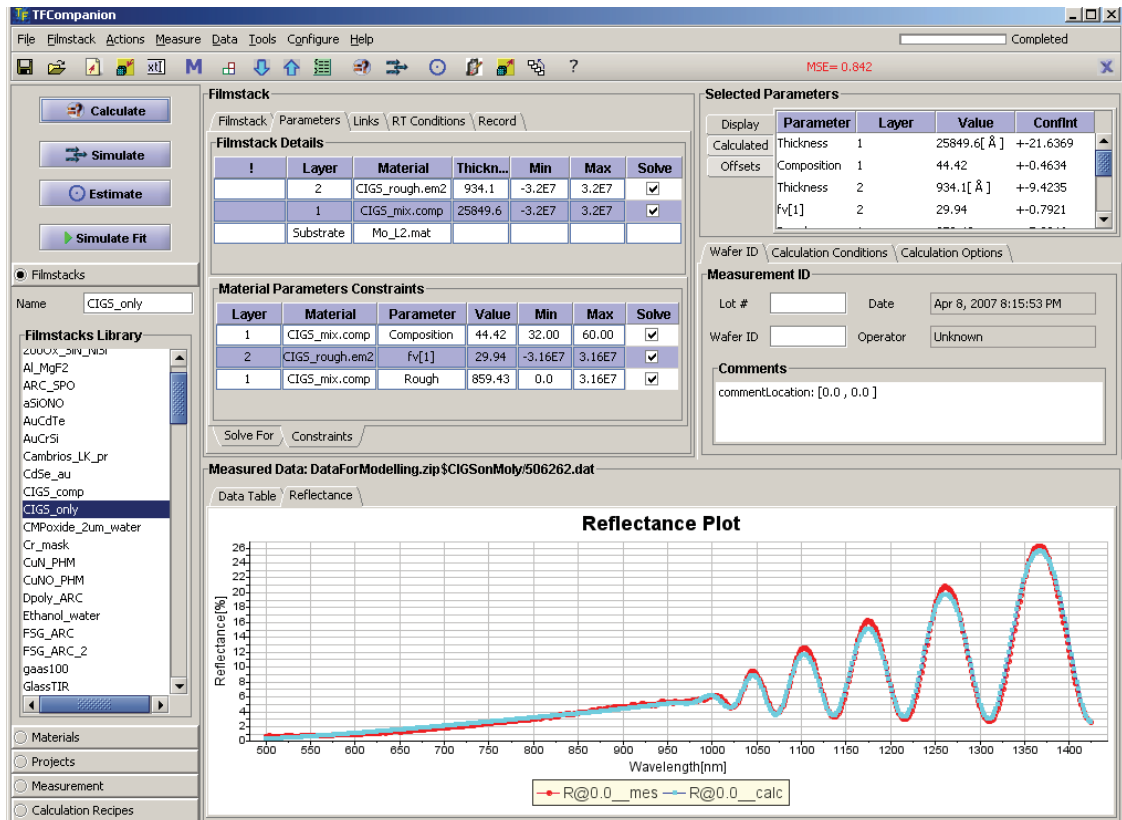
**Fig. 5. Case 2 : Measuring T,n,k of polySi.** The fit of model to measured data is much better. Thickness is 2.32 $\mu$ m

Case 2 (measurement of T,n,k) give the thickness of 2.32. $\mu$ m – this was found consistent with profilometry and spectroscopic ellipsometry results. Using traditional approach gives  $\sim 100$ nm error in thickness measurement.

### Example 3. Measurement of CIGS and CdS.

CIGS (Copper-Indium-Gallium-Selenide) is an important compound material used as an absorber in many thin-film solar cell structures. The typical solar cell filmstack is TCO/CdS/CIGS/Mo. Filmstack: CdS/CIGS/Mo is measured before top contact (TCO) deposition. It is important to determine both thickness and composition of CIGS. The surface of the CIGS is highly textured and the roughness has to be estimated and taken into account.

Results of the measurement in 400-1700nm range are shown on Fig. 6. In this measurement thicknesses of CIGS, composition of CIGS, thicknesses of CdS and surface roughness are determined simultaneously (4 parameters).



**Fig. 5** CdS/CIGS/Mo measurement (400nm-1700nm spectral range). Following parameters were measured: Thickness (CIGS)=2.5um, Composition(CIGS)=44%, Thickness(CdS)=0.93um, surface roughness (94nm).

**Example 4: Multilayer LiNbO3 filmstack on glass (backside reflectance correction).**

The following filmstack that is used for light projection application requires metrology control during the production process:

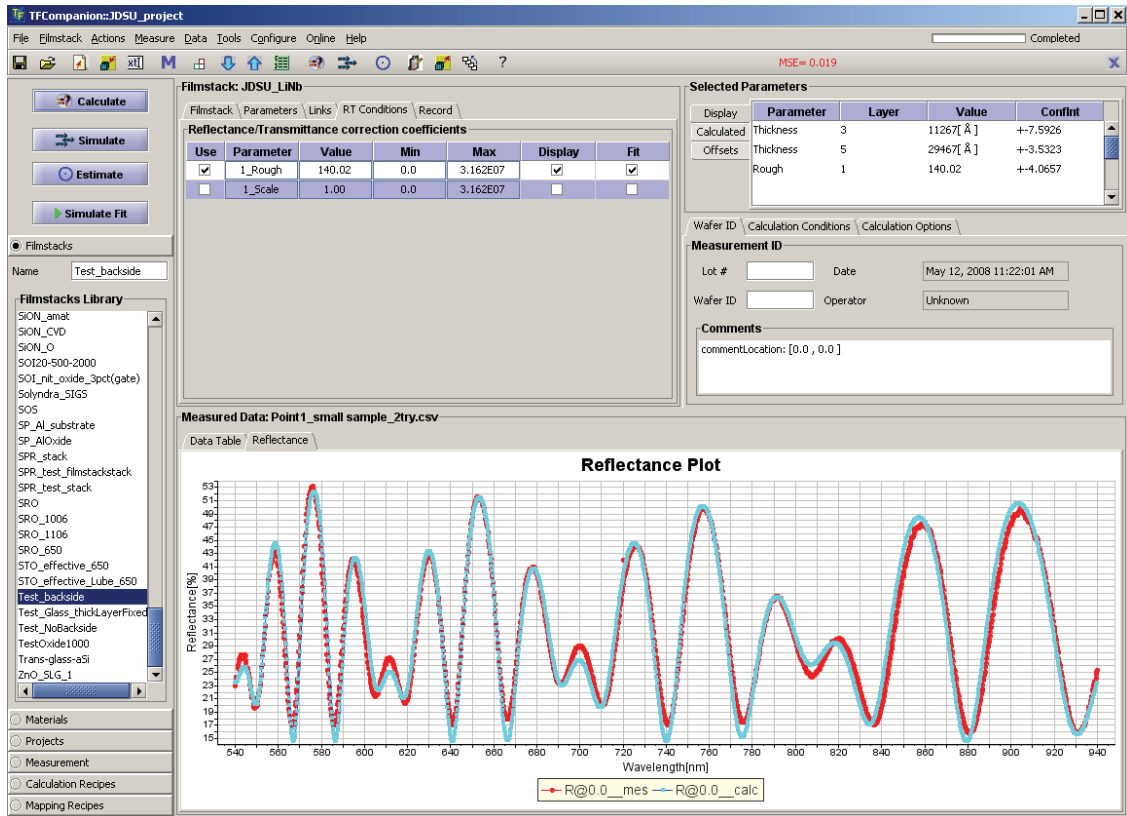
2um mgLiNbO3/0.5um SiO2/1.5um polymer/0.01um SiO2/900um cLbNbO3/ void

This filmstack presents several challenges:

- ✓ 900um cLbNbO3 substrate is transparent and backside reflectance need to be taken into account (it is also lightly absorbing)
- ✓ Light scattering caused by waveguide channels need to be taken into account
- ✓ Thicknesses of top layer and polymer can change in a wide range

For production control, two thicknesses (top layer and polymer) needed to be determined and monitored.

Typical measurement result is presented at Fig. 6



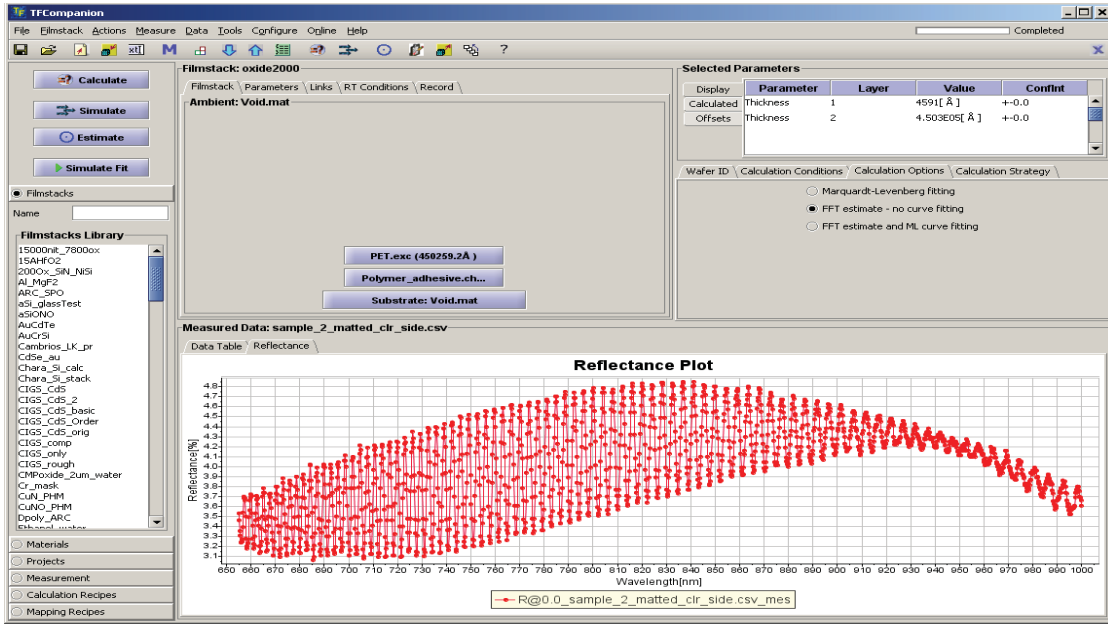
**Fig. 6 Measurement of LiNbO3 filmstack.**

Measured result (measured thicknesses are shown in red):

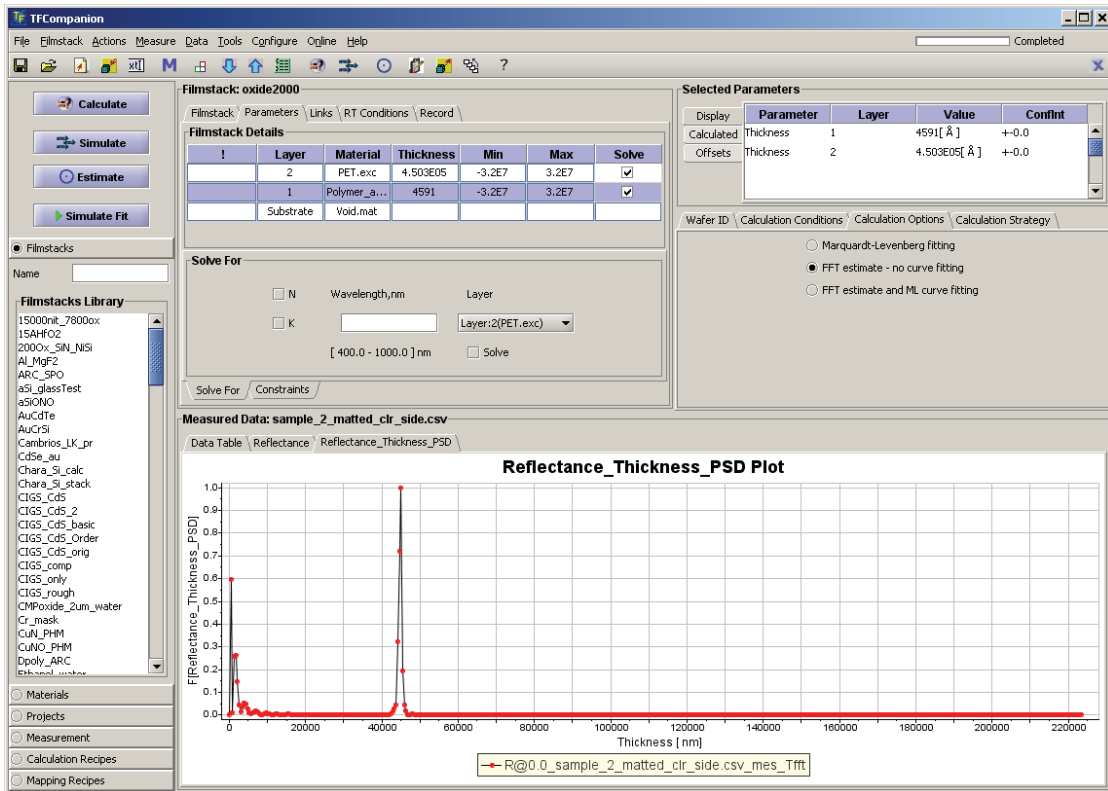
2.9467um mgLiNbO3/0.5um SiO2/1.1267um polymer/0.01um SiO2/900um cLbNbO3/void

**Example 5. Measurement of thick polymer stack.**

Two PET with adhesive layer(s) samples were measured. Sample 1 has two adhesive layers (adhesive/PET/adhesive), sample 2 has one adhesive layer on PET. Measurements were done in 700-1000nm range with 0.25nm resolution. Reflectivity of the samples was low ~ 3 to 4%. Measured reflectance spectra are presented on Fig, 7, 9 and show interference structure that can be easily analyzed as presented on Fig., 8, 10

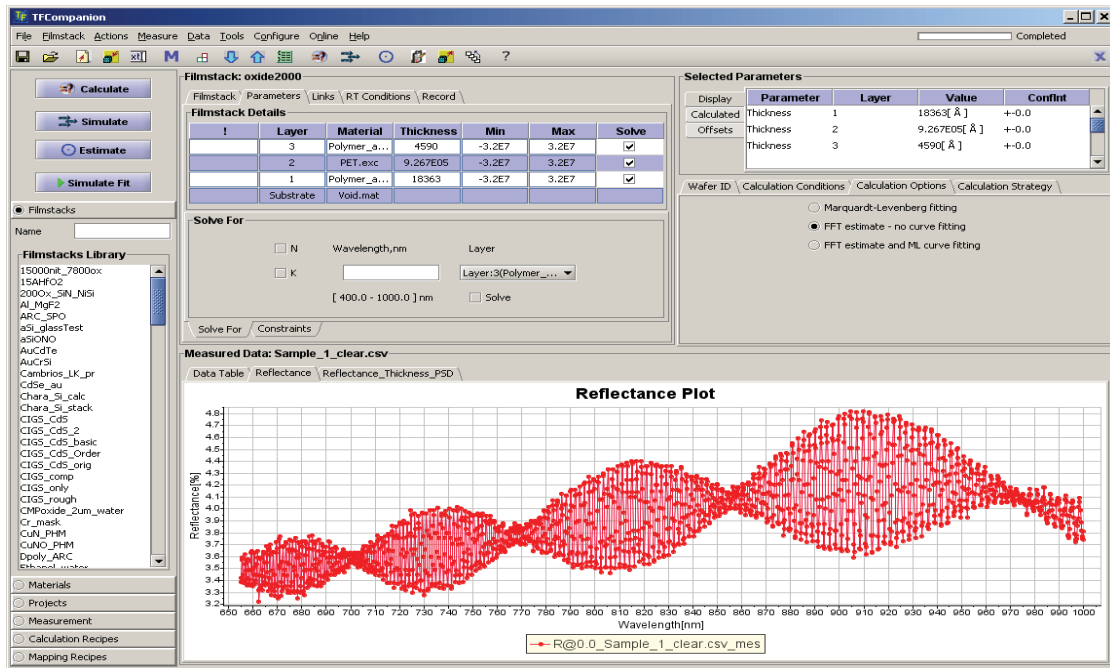


**Fig. 7** Sample #2 Reflectance spectrum. High frequency oscillations correspond to a thick PET layer (~45µm), low-frequency (half-period) corresponds to a thin adhesive layer

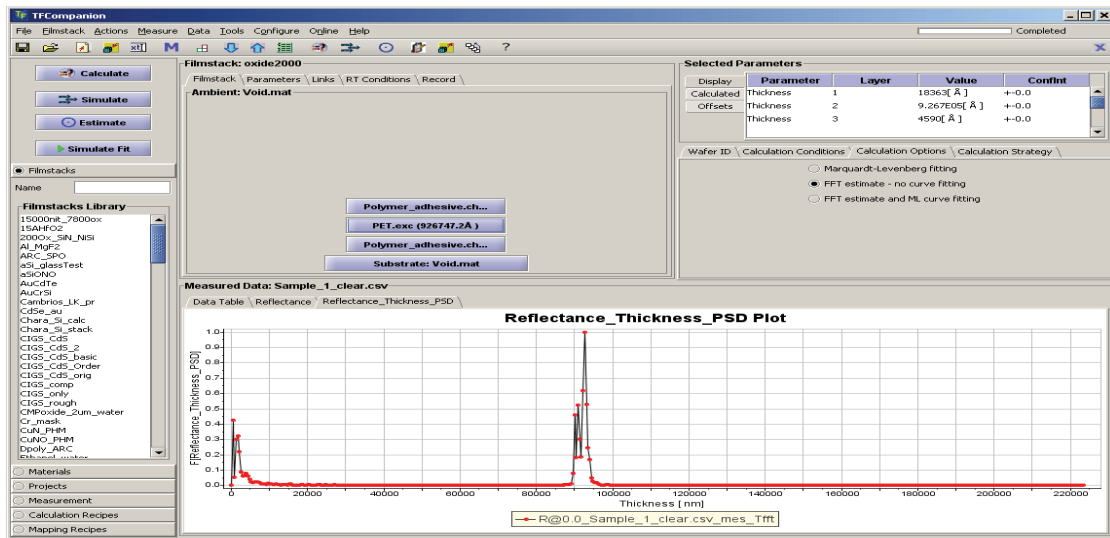


**Fig. 8** Sample #2. Analysis shows the presence of the two layer : PET (45 um) and adhesive (0.46um)





**Fig. 9** Sample #1 Reflectance spectrum. High frequency oscillations correspond to a thick PET layer (~ 92 $\mu$ m), slow variation (half-period) is similar to sample#2 and corresponds to a thin adhesive layer(0.46 $\mu$ m). The presence of the third layer -second adhesive (1.8 $\mu$ m)- is manifested by additional oscillation frequency



**Fig. 10** Sample #1 measurement analysis show three layers. (1.8 $\mu$ m adhesive/92.6 $\mu$ m PET/0.46 $\mu$ m adhesive)

## Example 6. Measurement of bandgap of SiCN

Using a Tauc-Lorentz dispersion approximation of the amorphous materials allows direct determination of the bandgap energy. In this example, SiCN sample (nominal 600nm SiCN/Si) was measured using MProbe UVVisSR (200nm -1000nm range). T,n,k and bandgap of the SiCN was determined from the fit to the measured data.

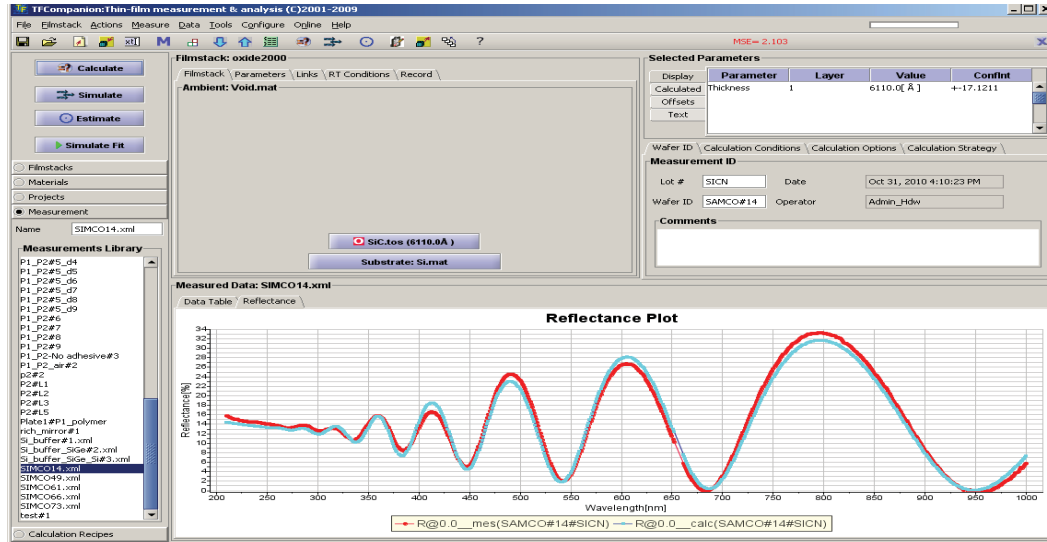


Fig. 11 Calculated vs. measured data fit for SiCN sample (611nm thickness)

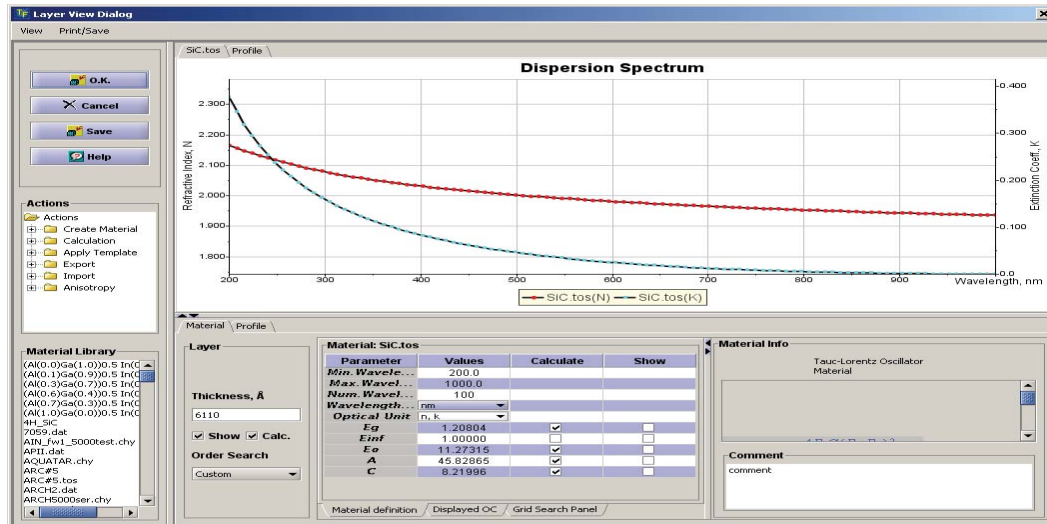


Fig. 12 n,k spectrum and bandgap (1.2eV) are determined from the fit to the measured data using Tauc-Lorentz approximation.

## Example 7. Measurement of TiO2

Titanium oxide optical constants depend on deposition conditions. Similar to SiN example (Example 1), using tabular values of standard stoichiometric TiO2 can result in thickness measurement error. This error is particularly difficult to detect if one measures only in the Vis range (400- 1000nm), because the fit to measured spectrum can be deceptively good. At the same time UV spectral range (200-400nm) is very sensitive to small change in stoichiometry because it affects absorption edge.

Amorphous TiO2 sample (TiO2 25nm/Si) was measured with MProbe UVVis system (200-1000nm). TiO2 dispersion was represented using a Harmonic oscillator model (2 oscillators) and  $n, k$  was determined from the fit to measured data.

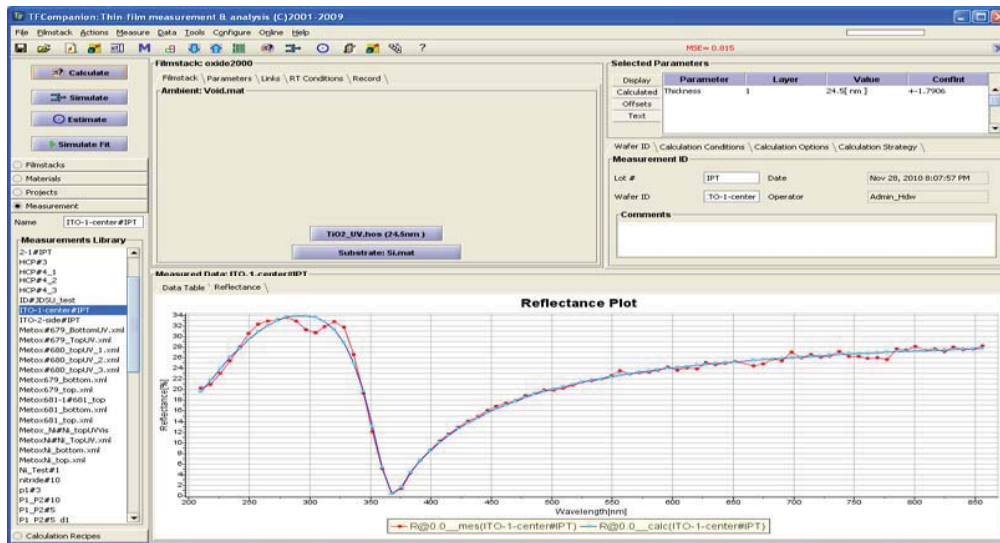


Fig. 13 Measured vs. calculated data fit for amorphous TiO2. (thickness 24.5nm)

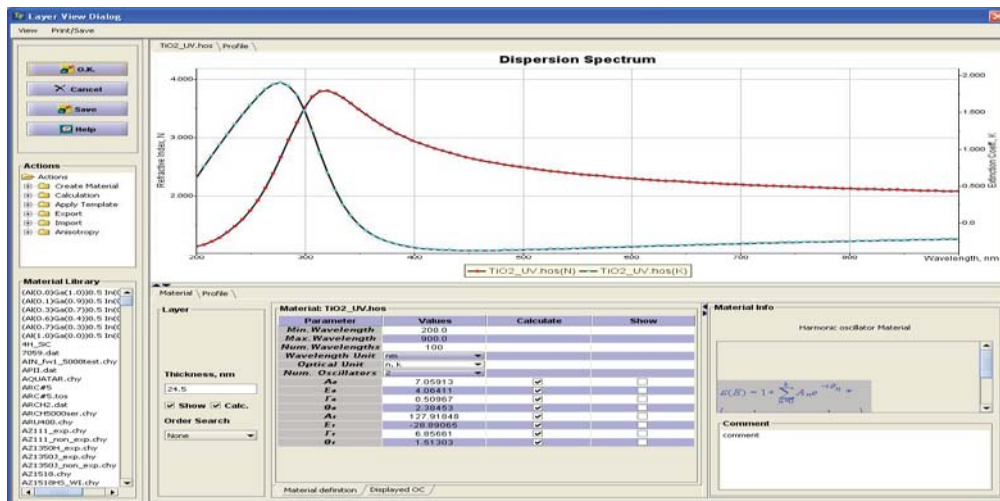


Fig. 14  $n, k$  dispersion of TiO2 is determined from the fit to measured data. TiO2 dispersion is represented using Harmonic oscillator model.

## Example 8 Measurement of ZnO

ZnO is an important material used in many applications, particularly as a TCO for thin-film solar and semiconductor laser heterostructures.

ZnO optical constant depend on stoichiometry and doping of the material. So, in many cases, it is imperative to measure  $n, k$  simultaneously with the thickness to get accurate results.

340nm ZnO/Si sample was measured using MProbe UVVisSR system in 200-1000nm wavelength range. ZnO dispersion was represented using Exciton dispersion model and  $T, n, k$  value were determined from the fit to the measured data.

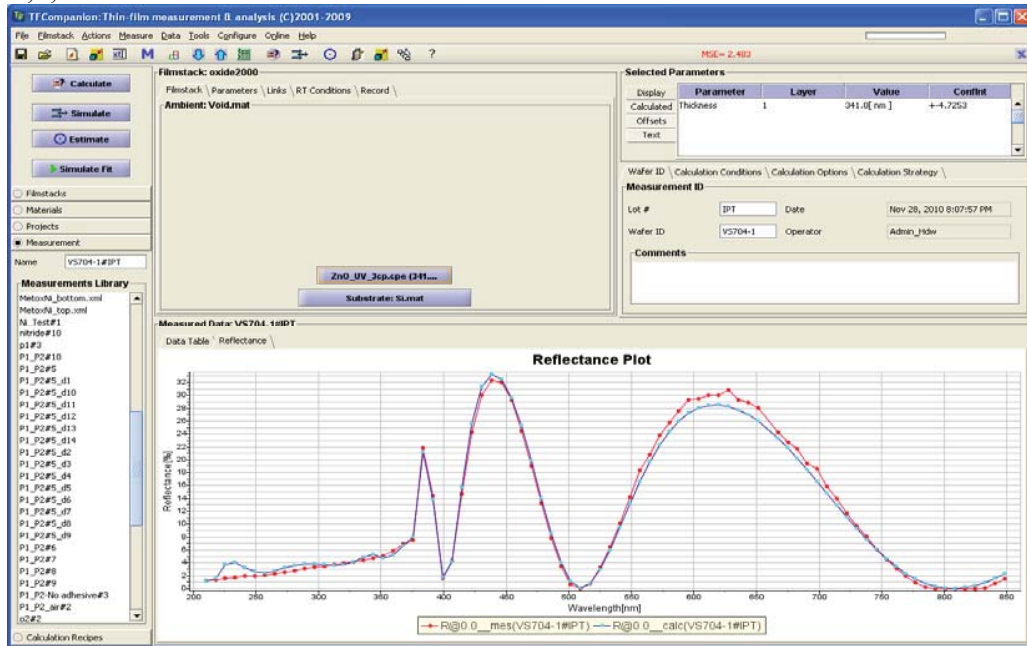


Fig. 15 Measured vs. calculated spectra fit for 340nm ZnO/Si sample.

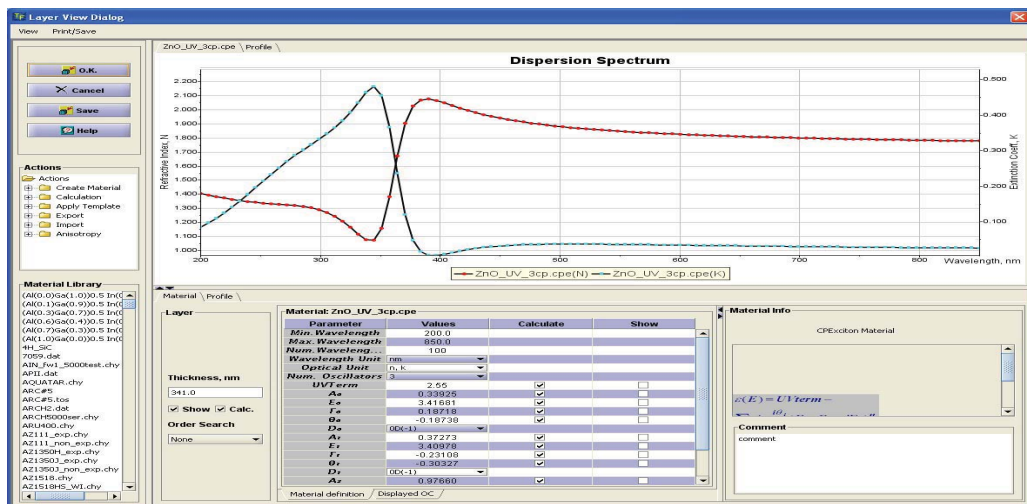
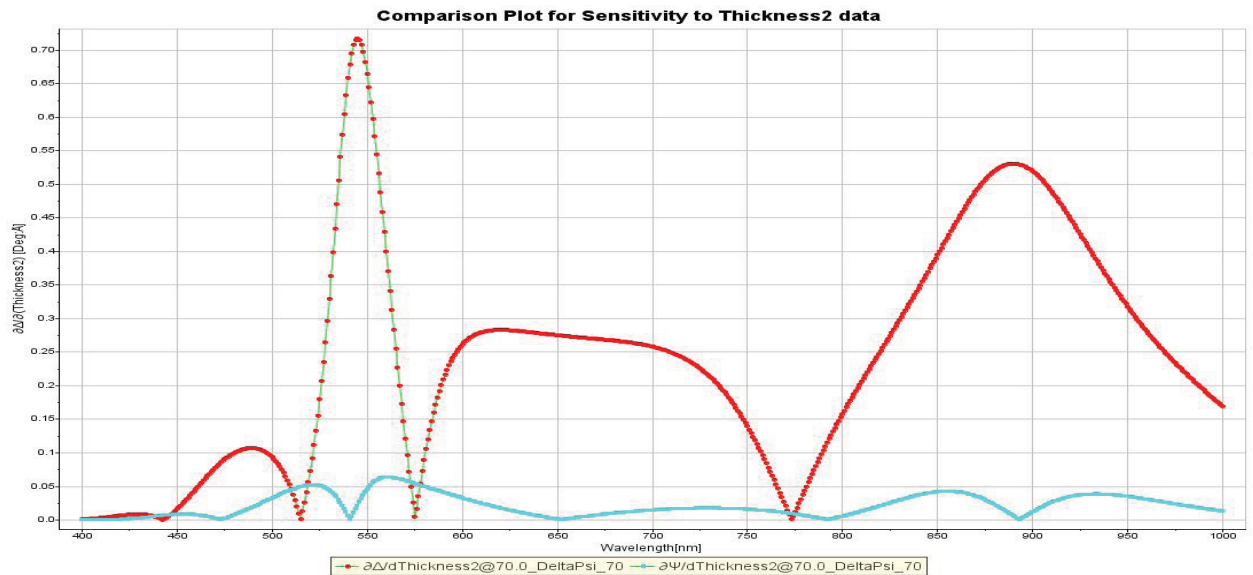


Fig. 16 ZnO  $n, k$  dispersion spectrum determined from the fit to measured data.

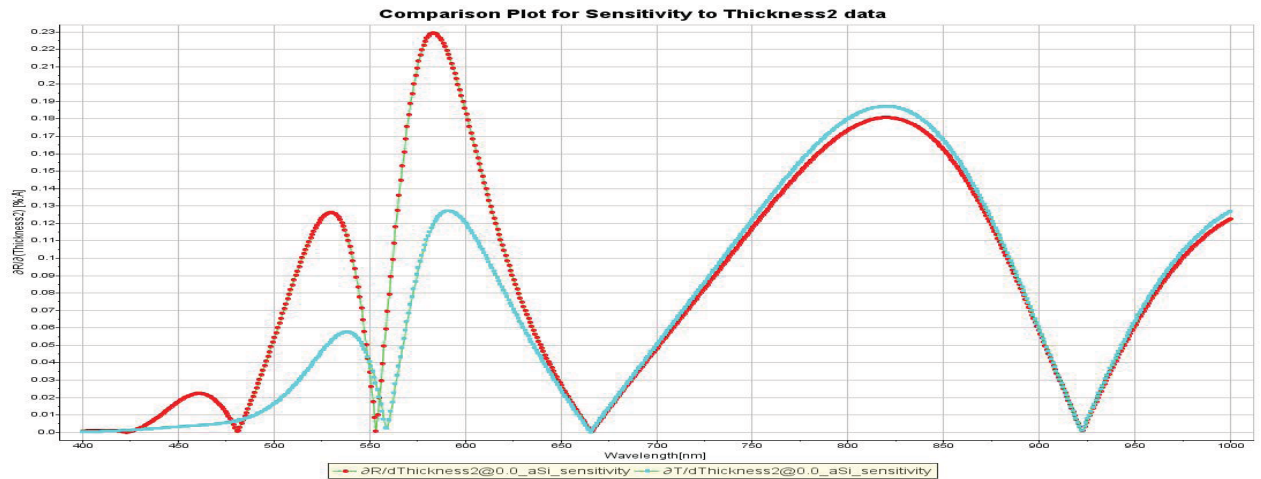
## Measurement sensitivity and precision

One of the advantages of using MProbe spectroscopic reflectometer system is a combination of very fast thickness measurement with high precision. The precision of 0.01 nm exceeds commercial spectroscopic ellipsometers performance and matches precision of the most high-end single- wavelength ellipsometers.

The common misconception is that spectral reflectance is significantly less sensitive to thickness. Simulated sensitivity of spectroscopic ellipsometry and reflectometry parameters to aSi thickness (thickness: 100nm) in 400nm-1000nm spectral range is presented on Fig. 11, 12. Delta (ellipsometry parameter) sensitivity is  $\sim 0.2$  deg/Å. (Maximum: 0.7 deg/ Å). Typical precision of Delta in spectroscopic ellipsometer is 0.1deg. This means the theoretically achievable thickness precision is 0.5 Å (or 0.15 Å maximum). At the same time MProbe spectroscopic reflectometer experimental precision is  $< 0.1$  Å. Average reflectance sensitivity of 0.2%/ Å corresponds to 0.02% of effective reflectivity precision.



**Fig. 17.** Sensitivity of Delta, Psi (ellipsometry parameters), to thickness of aSi. Average sensitivity:  $\sim 0.2$  deg/Å. (Maximum: 0.7 deg/ Å)

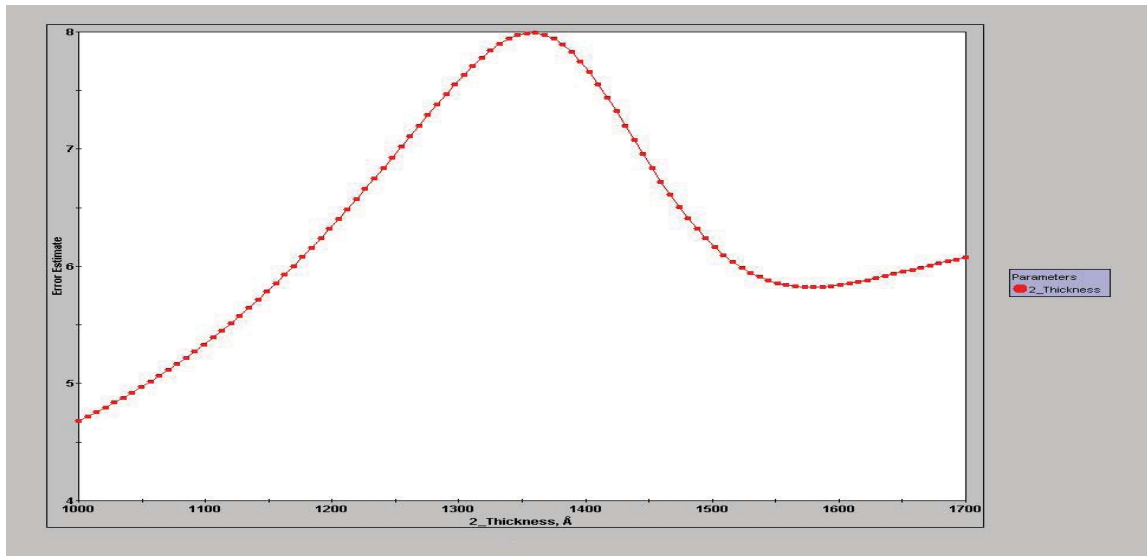


**Fig. 18** Sensitivity of spectroscopic reflectance to thickness of aSi.  
Average sensitivity:  $\sim 0.2\%/\text{\AA}$

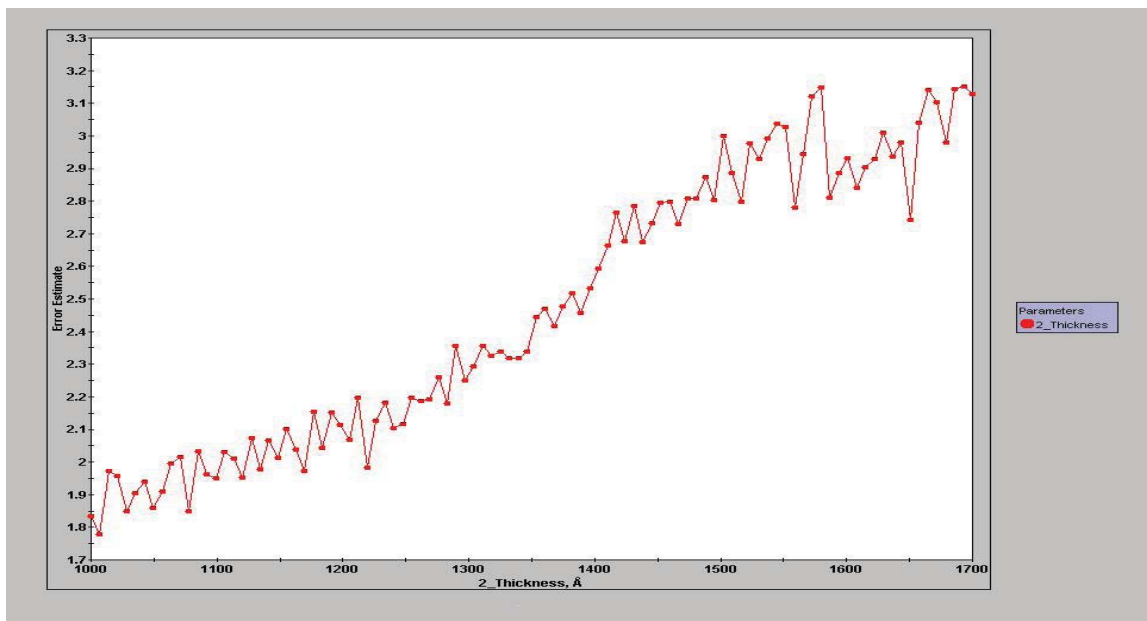
Simultaneous measurement of  $T$ ,  $n$ ,  $k$  affects (decreases) the precision for both ellipsometer and reflectometer system. Will spectroscopic reflectometer still be adequate?

To estimate the precision of  $T, n, k$  measurement we can use the same filmstack model and apply CMC (Covariance Monte-Carlo) approach [2,3]. CMC takes into account effect of the sensitivity and error propagation.

Results of the precision estimation for  $T, n, k$  measurement of 100-170nm aSi layer ( $n, k$  dispersion was represented using Tauc-Lorentz approximation) are presented at Fig. 19, 20. Precision is estimated as a function of aSi thickness. Results show that spectroscopic ellipsometry and spectroscopic reflectometry achieve comparable precision in 0.2% to 0.5%.



**Fig. 19 aSi layer: estimated precision of thickness measurement using spectroscopic reflectometry. Precision ~ 0.5% (5Å on 1000Å thickness). Calculated parameters: T,n,k (T+4 CL parameters).**  
 X axis: layer thickness, Y axis:  $1\sigma$  precision



**Fig. 20 aSi layer: estimated precision of thickness measurement using Spectroscopic Ellipsometry. Precision ~ 0.2% (2Å on 1000Å thickness). Calculated parameters: T,n,k (T+4 CL parameters).**  
 X axis: layer thickness, Y axis:  $1\sigma$  precision

## **Conclusion.**

Spectroscopic reflectometry is a powerful technique that can be used for a wide range of applications to measure both thickness and optical constants. Both spectroscopic reflectometry and spectroscopic ellipsometry have advantages and disadvantages and should be selected depending on application requirements. Spectroscopic reflectometry can be effectively used for thin-film solar applications, both in R&D and in production/inline monitoring and for many other critical applications

## **Reference:**

1. MProbe is a thin-film reflectometer system developed and manufactured by Semiconsoft, Inc. ([www.semiconsoft.com](http://www.semiconsoft.com))
2. L. Asinovski "Performance analysis of ellipsometer systems", Thin Solid Films, 455-6, pp.790 (2004)
3. L. Asinovski "Optical metrology: performance analysis: approach and metrics", Characterization and Metrology for ULSI Technology, AIP conference proceedings 788, p.314 (2005)

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