Measurement of Optical Constants (n,k) using MProbe

Measurement of spectroscopic reflectance allows determining both thickness and optical constants. It is easy to understand the basic reason of why it is possible. We are measuring reflectance amplitude and phase. Amplitude is measured directly at each wavelength but phase is derived from the interference fringes. As a result, we can determine thickness and n (refractive) index independently in case of the dielectric films. In case of absorbing materials (k>0), we have one additional condition – total absorption is a function of thickness, but n is independent of thickness.

In all cases, material is represented using parameterized material approximation i.e. optical constants are represented as a function of the wavelength.(dispersion relationship/equation). Dispersion relationship e.g. Cauchy, Tauc-Lorentz, etc. has several variable parameters (Cauchy – 3 parameters, Tauc-Lorentz – 5 parameters) that represent thousands of measured points. This allows to reduce the number of variable parameters.

Fig. 1. Light reflection from the filmstack diagram

Reflectance from a single layer filmstack can easily expressed using Fresnel equations:
\[ R = \frac{R_{12} + R_{23} e^{-i2\beta}}{1 + R_{12}R_{23} e^{-i2\beta}}; \]

where \( \beta = \frac{2\pi}{\lambda} nd \) (1)

\[ r_{12} = \frac{n_2 - n_1}{n_2 + n_1}; r_{23} = \frac{n_3 - n_2}{n_3 + n_2}; \]

\( \beta \) is optical phase. \( n_i \) is optical constant of the corresponding material and \( d \) – film thickness. The measured intensity \( I_m \) is \( R^2 \).

Practically, all cases of measuring \( n \& k \) and thickness simultaneously can be divided into two categories that we review separately:

1. Dielectric film (no absorption) that is relatively thick
   Most oxides, polymers are in this category
2. Films that have some absorption
   SiN, ZnO and many other materials are in this category

I. Dielectric films

Reflection spectrum from a thick oxide on Si wafer (Fig. 2) demonstrates two interesting properties:

a. Upper envelope \( R_T \) (line connecting the tops of interference peaks – constructive interference) is reflectivity of the bare Si: \( R_T = \left( \frac{n_{i-1}}{n_{i+1}} \right)^2 \), assuming that ambient is air (\( n=1 \))
   Low envelope \( R_B \) (line connecting the bottom of interference peaks – destructive interference) depends on the contrast between substrate and film refractive indices: \( R_B = \left( \frac{n_i - n_{i+1}}{n_i + n_{i+1}} \right)^2 \)

b. The distance between interference peaks depend on \( n \) and thickness. It can be readily shown from Eq.(1) that \( n_2 d = \frac{\lambda_i \lambda_{i+1}}{\lambda_{i+1} - \lambda_i} \); where \( \lambda_i \) and \( \lambda_{i+1} \) are wavelengths corresponding to adjacent interference peaks
Based on the properties (a), (b) we can conclude that thickness and refractive index can be determined independently. But it is also clear that film needs to be relatively thick. Thickness requirement will depend on the filmstack, film refractive index in particular. The good indications of how independent are parameters, is the correlation between the parameters.

<table>
<thead>
<tr>
<th>Thickness, nm</th>
<th>Correlation between $n$ and $d$</th>
<th>Conclusion</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.99</td>
<td>Cannot measure</td>
</tr>
<tr>
<td>200</td>
<td>0.20</td>
<td>Good/independent</td>
</tr>
<tr>
<td>2000</td>
<td>0.28</td>
<td>Good/independent</td>
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**Table 1.** Correlation between thickness and $n$ (refractive index) for different oxide thickness. Oxide R.I. is represented using Cauchy approximation. Correlation value is determined as an average correlation between Cauchy coefficients and thickness.
Measurement example: Polymer on glass

MProbe VisHR system used to measure in 700-1100nm wavelength range.

**Fig. 3** Polymer on glass. Fit between measured (RED) and model (Blue) data for polymer R.I.=1.582 at 800nm. Small amplitude of the model data shows that R.I. of the polymer is higher.
**II. Films with absorption**

Compared to dielectric films, absorbing films have additional parameter (extinction coefficient) that need to be determined. But there is also an additional constraint on the film thickness that allows determining extinction coefficient \(k\). Extinction coefficient is related to absorption (\(\alpha\)) as follows: 

\[
k = \frac{\lambda}{4\pi} \alpha,
\]

where \(\lambda\) is the wavelength of light. Intensity of light propagating in absorbing material material is decreasing exponentially: 

\[
I(d) = I_0 e^{-\alpha d},
\]

where \(I_0\) is intensity of the incident light, \(d\) thickness of film and \(I(d)\) is intensity of light at depth \(d\). At the same time, refractive index \((n)\) has no effect on the intensity.

In many cases, \(k > 0\) only in the part of the measured spectrum. For example, in the case of SiN, TiO2 and other metal oxides – material is dielectric in the Visible range and have absorption in UV range (Fig. 6)
Fig. 6  SiN dispersion represented using Tauc-Lorentz approximation. Absorption in UV range and dielectric film in the visible range. Measured dispersion is compared to dispersion of stoichiometric SiN.

We can again use correlation to access the effect of the thickness of the measurement of n&k and thickness independently (Table 2), as we did with oxide. We are using Tauc-Lorentz approximation (TLO) of SiN dispersion (Fig. 6). TLO coefficients affect both n and k together. So average correlation between TLO coefficients and thickness are indicative of combined correlation between n&k and the thickness.

We can notice that measurement is possible for the thinner films (20nm). Correlation is slightly higher for thicker films as compared to oxide.

<table>
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<tr>
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<td>0.82</td>
<td>Good/independent</td>
</tr>
<tr>
<td>100</td>
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<td>Good/independent</td>
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<tr>
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</tr>
<tr>
<td>1000</td>
<td>0.35</td>
<td>Good/independent</td>
</tr>
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Table 2  Correlation between thickness and n & k for different nitride thicknesses.
Measurement example: SiN on Si

Fig. 7 Using stoichiometric SiN optical constants to fit to measured data.

Fig. 8. SiN dispersion is represented using Tauc-Lorentz approximation. N & k values are adjusted to fit measured data. Comparison of the measured and tabular (stoichiometric) SiN optical constants see Fig 6.
III. Improving accuracy of n&k measurements.

How can we be sure that measured n&k are accurate? If we take two samples of different thickness and the same n&k will give a good fit in both cases – it is a good indication that n&k is accurate.

So, if we will use two or more samples of the same material but different thicknesses and analyze measurement results together – the accuracy of the n&k will be improved. Any correlation between n&k and thickness will be greatly diminished. Assuming, of course, that materials/optical constants in both samples are exactly the same. This approach is called “Multiple sample calculation”.

Fig. 9 Two sets of measurement (200nm and 500nm oxide) are matched with corresponding filmstacks
Fig. 10. Materials in both filmstacks are “linked” – this means that exact same material is assumed in both filmstacks and it has to fit both sets of measurements.

Fig. 11 After calculations – the best fit to both sets of data is achieved using the same material (the thicknesses are also calculated). The resulting n&k has a higher accuracy.