Invited Paper

Methods for optical modeling and cross-checking in ellipsometry and scatterometry

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ABSTRACT

Indirect optical methods like ellipsometry or scatterometry require an optical model to calculate the response of the system, and to fit the parameters in order to minimize the difference between the calculated and measured values. The most common problem of optical modeling is that the measured structures and materials turn out to be more complex in reality than the simplified optical models used as first attempts to fit the measurement. The complexity of the optical models can be increased by introducing additional parameters, if they (1) are physically relevant, (2) improve the fit quality, (3) don't correlate with other parameters. The sensitivity of the parameters can be determined by mathematical analysis, but the accuracy has to be validated by reference methods. In this work some modeling and verification aspects of ellipsometry and optical scatterometry will be discussed and shown for a range of materials (semiconductors, dielectrics, composite materials), structures (damage and porosity profiles, gratings and other photonic structures, surface roughness) and cross-checking methods (atomic force microscopy, electron microscopy, x-ray diffraction, ion beam analysis). The high-sensitivity, high-throughput, *in situ* or *in line* capabilities of the optical methods will be demonstrated by different applications.

Keywords: Ellipsometry, Scatterometry, Cross-checking, Comparative Study, Optical characterization, Thin films

1. INTRODUCTION

Thin film characterization methods are of primary importance in numerous key technologies like microelectronics, photovoltaics or sensorics. Vertical compositions can usually be determined by removing the films (e.g. by sputtering) during surface-sensitive measurements (such as secondary ion mass spectrometry, sputtered neutral mass spectrometry, X-ray photoelectron spectrometry, Auger electron spectrometry, glow-discharge optical emission spectrometry, glow-discharge mass spectrometry, Raman depth profiling), by non-destructive depth-profiling techniques (such as Rutherford backscattering spectrometry, elastic recoil detection analysis, angle-dependent soft X-ray emission spectroscopy, grazing incidence X-ray diffraction, ellipsometry), or by cross sectioning techniques (such as electron microscopy, scanning Auger electron microscopy, time-of-flight secondary ion mass spectrometry, Raman mapping).[1] From the perspective of the above list and the features of thin film metrologies, the advantages of optical techniques like ellipsometry and scatterometry are three-fold. (1) They allow a quick measurement. Ellipsometry is typically capable of measuring a broad spectrum (≈200-1700 nm) within less than one second, whereas the other destructive (layer removal by sputtering) and cross-sectional methods require minutes or rather hours (e.g. in case of electron microscopy) for measuring in one point. (2) The second

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important feature is the sensitivity, especially in terms of vertical resolution, or geometrical parameters in case of scatterometry. Also, the lateral scale of characterization can vary from the diffraction limit (down to about one micron) to even meters. (3) Finally, the speed and sensitivity allows measurements on large surfaces[2,3] and *in situ* or *in line* characterizations during thin film growth,[4–6] processing[7–14] and manufacturing.[15,16]

However, there is also a major challenge: the quantification is made through optical models and numerical methods, and therefore the interpretation of the results is not straightforward.[17–19] Methods like the above mentioned complementary techniques,[1] extended by scanning probe methods like atomic force microscopy (AFM) or scanning tunneling microscopy, are often used for cross-checking and verification. As shown below, these techniques also have drawbacks, such as different information depths. In this paper we show several results and point out some challenges, mainly focusing on our own results as examples.

2. OPTICAL METHODS

Some of the widely used optical surface and thin film characterization methods are reflectometry,[20,21] ellipsometry[17–19] (polarimetry in general) and scatterometry.[22] All these methods measure the change of electromagnetic radiation during reflection from or transmission through the investigated sample. The advantage of ellipsometry over reflectometry is that the input intensity does not have to be known, and the sensitivity is higher due to the capability of measuring the phase change between reflections polarized parallel and perpendicular to the plane of incidence. Ellipsometry can be considered as a special kind of interferometry, in which the reference beam is that of the orthogonal polarization. Scatterometry provides additional information if the sizes of characteristic surface features or structures are comparable or larger than the wavelength used for the characterization. A new possibility is the combination of the two methods,[23] although ellipsometry has already been used for scattering or diffracting samples in specular or normal-incidence configurations.[24–27] The high speed of optical methods can also be utilized in large area mapping of thin film properties,[2,3,28] e.g. photovoltaic[29] or display panels. Currently a 40-point spectroscopic line-scan can be made in 10 s, and the near-future aim is a spectroscopic map of a 60 cm by 120 cm photovoltaic panel within 1 min.[29]

An emerging powerful method is Fourier scatterometry, which measures the light scattered from the focus of a large numerical aperture objective by imaging the Fourier plane.[30,31] Consequently, the major advantage of the method is that a large range of scattering and azimuth angles (0-64 and 0-360 degrees for reflection and azimuth angles, respectively, with a numerical aperture of 0.9) can be measured quickly and simultaneously. A great challenge is currently the quick calculation based on the large number of acquired measurement data. Improved sensitivity has been demonstrated by utilizing a scanning focused spot,[32–38] interferometry[39,40] or ellipsometry.[23]

3. MODELING

Being indirect methods, optical techniques like reflectometry, scatterometry or ellipsometry require some *a priori* information on the investigated structure, which helps to build proper optical models. When investigating complex samples (e.g. involving special features like the line edge roughness,[41] overlayer thickness and bottom rounding,[42] vertical inhomogeneity[43] or the parameterization of the dielectric function for spectroscopic measurements[44]) the number of fit parameters increases, and a reliable fit approaching the global minimum of the system can only be achieved by sophisticated procedures[45] like the maximum likelihood method,[46] random global search,[47] simulated annealing or genetic algorithms.[48]

The sensitivity of the parameters can be checked by uncertainty analysis.[23,32,49] In case of spectroscopy and characterization of material properties, the parameterization of the dielectric function is a major issue from which a lot of technologically important material properties can be obtained, like for the case of polycrystalline semiconductors.[50,51] Also in scatterometry, using different wavelengths in a broad range can increase the accuracy, reliability and the number of fit parameters.[52]

For the modeling of structures, the most widely used approach is to think in terms of stratified systems composed of layers with plane and parallel boundaries, and to calculate the optical response using the transfer matrix method[53] or (in case of diffracting samples) by the rigorous coupled wave analysis (RCWA).[14,26,27,54,55] Finite element (FEM)[56,57] and finite difference in time domain (FDTD) methods[58–60] are also rapidly emerging.

In terms of materials, there is a wide range of parameterizations depending on the electron structure (mostly categorized as dielectrics, metals or semiconductors).[61,62] Optical parameter reconstruction requires a lot of computation, therefore, grid computing (as applied in Ref. 63) or using graphics processing units[64,65] are becoming more and more important.

4. METHODS FOR CROSS-CHECKING

Because of their indirect character, the validation of optical methods is of primary importance. It means that the method has to be traceable to a reference standard.[66] Although a reference standard is a stable and highly reproducible structure,[67] it is suitable for validation only when measured and cross-checked with other reference methods.[66] As a primary aim, it is also crucial to achieve accurate optical measurements at the industrial level.[68]

There are numerous thin film characterization techniques including depth profiling like secondary ion mass spectrometry, X-ray photoelectron spectrometry, Auger electron spectrometry, glow-discharge optical emission or mass spectrometry, Raman depth profiling, non-destructive techniques such as Rutherford backscattering spectrometry, heavy ion elastic recoil detection, angle-dependent soft X-ray emission spectroscopy, grazing incidence X-ray diffraction or ellipsometry. Finally, there are the most traditional cross-sectioning techniques like scanning electron microscopy, scanning Auger electron microscopy, or Raman mapping.[1] Table 2 of Ref. 1 gives a nice overview of the main characteristics of a large number of thin film profiling techniques. Most importantly, there were significant deviations observed between the different methods by measuring on the same structure, which also pointed out the importance of validation, and the significance of suitable reference and calibration structures and methods.

5. PERIODIC SURFACE STRUCTURES

The most frequently applied structures used for the validation of scatterometry are two-dimensional gratings evaluated by RCWA[54,55] or FEM[57] using goniometric scatterometry,[52,69] Fourier scatterometry[30–32] or ellipsometry.[14,25–27] Most of these studies use scanning electron microscopy (SEM) and AFM for cross checking. However, the measurement of side-wall angles and corner roundings are challenging with both methods, for which only transmission electron microscopy (TEM) can be used as the most reliable reference method.

Measurement of height and side-wall angles are major weaknesses for SEM and AFM, respectively. Even with TEM, a possible lateral inhomogeneity remains a great problem (also for line edge roughness characterizations[31]), since the spot size of the optical measurements are usually much larger than the TEM image area. In Ref. 69, the deviation between the different SEM approaches was comparable with its deviation from the optical results. From top view SEM, a critical dimension deviation of approximately 3 nm was claimed with sophisticated signal analysis for line widths of ≈100 nm. A typical agreement within several nanometers is obtained between the scatterometric and electron microscopic results[37–39] (with accurate height values measured only by AFM) and also between different scatterometric approaches (Table 1), slightly depending on the methods for fitting and modeling,[70] e.g. considering a possible unintentional surface overlayer.[38,71]

There is a large potential in the optical characterization of other two- or three-dimensional periodic structures from biological[72] or bio-inspired[73,74] to special fiber[75] or sensor structures.[76,77] In all these, the measurement on small areas (like single scales of butterfly wings[78]) or non-uniform surfaces is an important challenge, as well as the capability of the proper alignment of the sample surface. Efficient and powerful calculation methods[53–55,57,60,79] with sophisticated algorithms[45,46,48,63] are also becoming increasingly needed.

6. SURFACE ROUGHNESS AND ULTRA-THIN LAYERS

The high surface sensitivity of ellipsometry makes it especially suitable for roughness measurements for both surfaces[80] and interfaces[81–83] on the nanometer scale. Besides other sophisticated methods like the Rayleigh-Rice theory,[84] the most popular and robust method for surface roughness measurement is the effective medium approximation (EMA).[80,85–87] Although a good correlation was revealed between the root mean square roughness measured by AFM and the thickness of the roughness layer measured by ellipsometry using the EMA, some effects like the window size in AFM have to be taken into account for a proper comparison and quantification (Fig. 1).

Table 1. Best-fit reconstruction of Si gratings using deep ultraviolet (DUV) scatterometry and Fourier scatterometry, utilizing the maximum likelihood estimation (MLE) and the non-linear least squares fit. The parameters of the grating are listed in the first column. [Reprinted from the SPIE Proceedings 9132 (2014) 913208-1, Endres et al., "Measurement comparison of goniometric scatterometry and coherent Fourier scatterometry".]

Reconstruction parameter	**DUV scatterometer**		**Fourier scatterometer**
	MLE	Nonlinear least squares	Nonlinear least squares
Middle CD [nm]	301.5±1.5	277.5±1.2	277.0
Height [nm]	361.0±1.0	370.8±0.5	365.0
Side wall angle [°]	83.8±0.3	81.9±0.2	90.0
Oxide layer thickness [nm]	4.9±0.5	2.77±0.28	5.0
Bias value [nm]	-		150

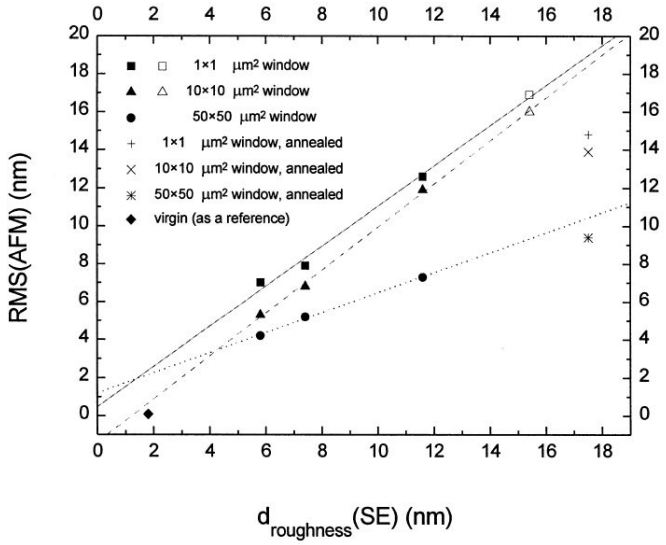

Figure 1. Root mean square (RMS) roughness measured by atomic force microscopy (AFM) correlated with the roughness determined by spectroscopic ellipsometry (SE), for different AFM window sizes.[87] [Reprinted from Thin Solid Films 315 (1998) 186, Petrik et al., "Surface roughness measurement on polysilicon produced by low pressure chemical vapor deposition using spectroscopic ellipsometry and atomic force microscopy". Copyright 1998, with permission from Elsevier.]

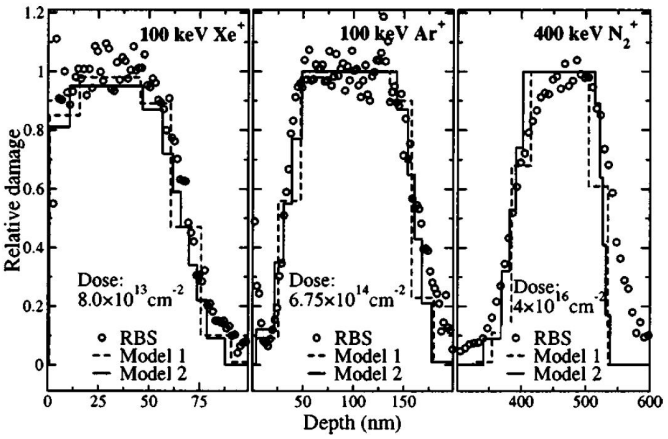

Figure 2. Damage depth profiles in Si, induced by implantation of Xe^+, Ar^+ and N_2^+ ions at different energies (see graphs) measured by spectroscopic ellipsometry (lines) verified by Rutherford backscattering spectrometry (RBS). The optical models were based on coupled half-Gaussians[97,98] with equal sublayer thicknesses (Model 1) or sublayer thicknesses inversely proportional to the slope of the profile (Model 2,[92]). Reprinted from the Journal of Applied Physics 93 (2003) 1987, Petrik et al., "Ellipsometric characterization of damage profiles using an advanced optical model".

In case of ultra-thin (several nanometers) layers the interface roughnesses[82,83] and the surface contamination are crucial questions. It was shown that native oxide covered samples acquire 0.1 to 0.2 nm of organic contamination within two hours stored in closed but nonvacuum conditions. Subsequently, another 0.2 to 0.5 nm layer is deposited, which is saturated in approximately in one week.[88] The thickness in that study was a kind of 'SiO_2-equivalent' thickness – the accurate analytical measurement of low surface contamination is also very challenging.[89] The above contamination layer is the reason why ellipsometry usually slightly overestimates the thicknesses of ultra-thin layers when compared with methods measuring in vacuum (see the comprehensive study involving ion beam, X-ray, electron and optical investigations in Ref. 90).

7. DEPTH PROFILING IN SEMICONDUCTORS

For optical techniques accessing higher photon energies (e.g. the direct interband transition energies of 3.4 and 4.2 eV in Si), the long range order and minute changes in the crystal lattice can be measured with high sensitivity. This is the reason why ellipsometry can be applied for the measurement of polycrystalline and ion implanted semiconductors. Damage profiles can be determined from the optical measurements using multilayer models with the EMA and the transfer matrix method. Besides TEM, an accurate verification method for damage profile measurement is the ion beam analysis (when the sample is single-crystalline or the grains of the polycrystal are not randomly oriented[91]) irradiated from channeling directions. Fig. 2 demonstrates the agreement in damage profiles measured by ellipsometry and Rutherford backscattering spectrometry (RBS).[92] In case of very thin layers, medium energy ion scattering is even more accurate than RBS.[93,94] The combination of RBS with ellipsometry is also a powerful method for density measurements, because ellipsometry provides an accurate thickness value, whereas RBS delivers the number of atoms per unit surface.[95]

In case of near surface cavities in Si, the high sensitivity is ensured by the large optical contrast between void and Si. In this case, TEM is the most suitable verification method. We have obtained good agreements in different studies.[63,96]

Finally, it should be pointed out that the decreased penetration depth at direct interband transition photon energies is not only a problem, but it can also be utilized for depth scanning, when properly choosing the wavelength range used for the optical characterization (Fig. 3). By a systematic scan of the wavelength range, the penetration depth can be varied in a controlled way, which allows a model-independent direct depth scan. This might open new directions in the optical characterization of vertically non-uniform absorbing films.[99]

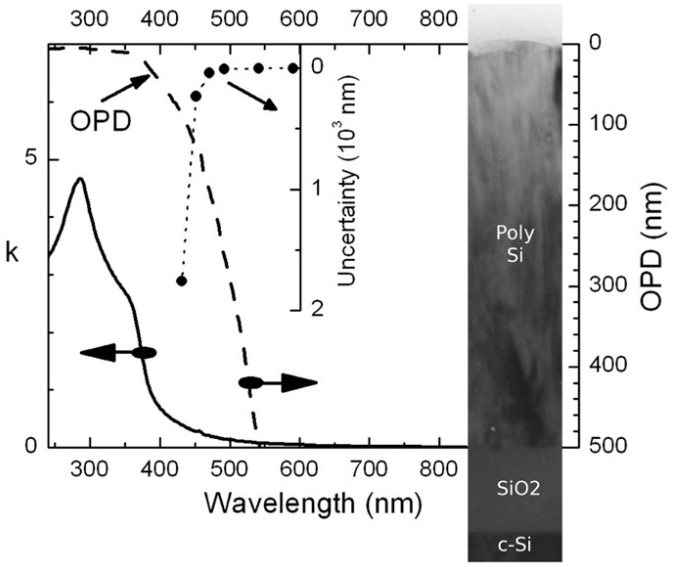

Figure 3. Extinction coefficient (k) and optical penetration depth (OPD) of a polycrystalline silicon layer (see TEM image on the right-hand side) as a function of the wavelength. The uncertainty of the fitted thickness is also shown as a function of the cut-off wavelength.

CONCLUSIONS

We have shown some aspects of optical modeling and cross-checking in ellipsometry and scatterometry. Proper quantification and the need for reference samples remain major challenges in the future, not only for optical but also for most other metrologies.[1,89,90]

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