### Appraising the Extensibility of Optics-Based Metrology for Emerging Materials

B. M. Barnes, M.-A. Henn, M. Y. Sohn, H. Zhou, and R.M. Silver

Nanoscale Device Characterization Division, Physical Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA

> To advance computational capabilities beyond conventional scaling limitations, novel device architectures enabled by emerging materials may be required. Optics-based methodologies, central to modern-day process control, will be pursued by the nanoelectronics industry to interrogate these devices as optics are inexpensive, nondestructive, and fast. As geometrical and material complexity define new metrology requirements, these should be considered relative to the broader challenge of perpetuating optical methods for deepsubwavelength features. Using examples from our group and from others, the tailoring of the illumination conditions, sample, collection path, and data analysis are emphasized for model-based quantitative measurements. The successful fitting of structures comprised from these emerging materials will require the accurate determination of material optical constants, which may be both thickness dependent and anisotropic. Atomistic models such as tight-binding calculations or density-functional theory are potential approaches for understanding the dielectric function of these materials.

# Introduction

Optical methods are successfully solving critical measurement challenges in conventional nanoelectronics, but anticipated increases in device and materials complexity will assuredly require advances in current methodologies (1). It is likely that emerging computation architectures (2) will integrate emerging materials to achieve effective computational performance gains like those previously realized in microelectronics and nanoelectronics due to transistor scaling as described by Moore's Law. To understand how optics-based metrology techniques might respond to the inherent challenges from these materials, previous solutions for extending optical methods for complementary metaloxide-semiconductor (CMOS) materials should be reviewed. Results from our laboratories at the National Institute of Standards and Technology (NIST) and elsewhere foreshadow potential industrial approaches for dealing with emerging materials in this key context. A central theme in our research has been the tailoring of the measurement conditions such that the full three-dimensional (3-D) scattered field yields as much information as practicable about the devices of interest, which are sized well-below the conventional diffraction limit. Industry has augmented solutions developed at NIST and by other measurement scientists, and continued progress is required to enable the optical measurement of smaller, complex, heterogeneous devices. This paper describes multiple experimental characteristics available for optimizing optical scattering for metrology with examples, including a description of current data analysis approaches that complement these approaches. Challenges specific to certain emerging materials are identified, and atomistic simulations are suggested as one potential response to these challenges.

### Tailoring the Experimental Conditions to Optimize Dimensional Metrology

Optical methods are fast, non-destructive, and can cover relatively large areas intrinsically parallel, yielding quick measurements of reflected and scattered intensities off samples of interest. In the microscale, imaging optics can yield the width of features (*e.g.*, a bacterium) directly if the dimensions of the field-of-view have previously been characterized. However, in modern nanoelectronics, the heights of conformal and thin films are integral to device performance while features are also sized well-below conventional resolution limits. To determine dimensions using optics-based measurements, a geometric model must be chosen that closely replicates the nominal dimensions and composition of the features or thin films. The fundamental physics underlying the scattering or reflectivity measurements must be accurate while also yielding successful fits between simulated and measured intensities. Several iterations in which the geometry's parametric values and material optical properties are varied may be required to determine a solution. Notably, the solution may not be unique and furthermore, one may have difficulties distinguishing changes between or among parameters due to parametric correlations. These correlations obscure the parametric values and uncertainties of various heights, widths, and optical properties (e.g., n & k).

Optics-based metrology for nanoelectronics is greatly aided by prior knowledge of nominal materials composition, nominal films thicknesses, and nominal patterned features sizes designed to yield specific electrical characteristics (*e.g.*, transistors) (3). Such device designs are repeated periodically with great precision, potentially allowing for higher-order optical diffraction (if the periodicity, *p*, is not far smaller than the optical wavelength,  $\lambda$ ). Although these technological designs are configured to enhance *computational* performance, there still exist several opportunities to best enhance the three-dimensional *scattered electromagnetic field* at the sample to optimize the *dimensional* measurement and *optical properties* characterization of these films and features.

Several components of an optics-based measurement can be tailored to enhance the desired metrology of the device. The first components are bundled in "illumination engineering" (4), the incident light approaching the sample. These factors include the incident beam's polarization state, its wavelength, and its angle of incidence. These can be probed through simulations prior to measurement. If high-magnification microscopy is included, then the position of the sample relative to the incident beam (*e.g.* focus position, sample tilt) may also be optimized (5). Although the areas available for metrology targets within the technologically defined layout are relatively small, additional opportunities may exist to improve measurements using combinations of target design and optical methodology (6). Furthermore, one may also optimize the collection numerical aperture (CNA) and additional polarization filtering. Even after the intensities are collected, data processing can be optimized as well. As there can be significant interplay among these multiple potential components used to modify the resulting scattered field, each has to be assessed in concert with the others in order to successfully quantify the desired measurands.

#### Reflectometry, Ellipsometry, and Scatterometry

Selected experimental characteristics are optimized for metrology in three important nonimaging optics-based measurement methods: reflectometry, ellipsometry, and scatterometry. These three may be viewed as a succession of ever-improving measurement capabilities that have enabled contemporary characterization of complex nanoelectronics devices. Optical reflectometry in this definition indicates an incident beam reflected off a surface with no additional scattering or diffraction, either due to a lack of features on the surface or because their periodicity  $p \ll \lambda$ , the incident wavelength. Reflectometry can be goniometric (i.e., variation of incident angle) or spectroscopic (i.e., variation of incident wavelength) (7). Matrix methods that invoke straightforward analytical solutions through Fresnel equations and Snell's law are all that is required in many situations to interpret experimental data for reflectometry. In ellipsometry, the incident polarization state is varied and changes in both intensity and polarization are monitored in the collection path (8). Figure 1 illustrates the basic components of a reflectometer and shows added components that would enable ellipsometry. Many other configurations exist, see (9). The addition and variation of these polarizing elements for ellipsometry yield additional data about the sample through several realizations of the reflected field. Empirical models of ellipsometric data are useful for extracting key materials details such as film thickness and optical parameters of the materials (9).

Note, while ellipsometry is used widely on thin-film stacks that yield only reflection, a technologically relevant form of ellipsometry is now being applied not just to reflecting samples but also to samples that both reflect and scatter light. Although often only the specular reflection is captured, introduction of additional elements (e.g., quarter-wave plates) enable not just measurements of intensity and polarization changes but also depolarization. These Mueller-Matrix Spectroscopic Ellipsometers (MMSE) can utilize full electromagnetic simulations to determine the parameterized geometry, materials thicknesses, and their optical parameters. Additional information about MMSE can be found in Ref. (10).



Figure 1. Schematic diagram of a reflectometer (darker-shaded elements) shown with augmented optics (lighter-shaded elements) to permit ellipsometry. Adapted from (9).

Scatterometry is a more general term applied to optical instruments that require modelbased metrology to determine the specular reflection from samples that both scatter and reflect light, such as periodic arrays of transistors (11-13). One may say that scatterometers are optical instruments that encompass scatterometry, ellipsometry, and reflectometry (14). In a simulation study conducted by our group and other colleagues at NIST, the differences between goniometric and spectroscopic scatterometry were presented (15). Angle scans proved sensitive to a given parameter but often with significant correlations among the several parameters. Parametric correlations proved to be greatly reduced when using spectroscopic data, and in nanoelectronics fabrication, spectroscopic scatterometry has become integral to fabrication and process control (1, 16).

#### Scatterfield Microscopy

Despite these noted advantages of spectroscopic scatterometry, there are certain tradeoffs to utilizing a non-imaging system. For instance, scatterometry measures the average line width and height across an area illuminated by the incident beam. Reductions in beam size have been pursued, with microspot sizes in spectroscopic ellipsometry reported in 2009 between 50  $\mu$ m to 25  $\mu$ m, depending on wavelength (17) with recent reports at 15  $\mu$ m (18). Such reductions are critical as in general, the simulations for scatterometry assume an infinite grating. Stated differently, the spot size is fully within a specialized designed scatterometry target, and as the spot size decreases, the minimum area for the target also decreases. However, such scatterometry targets remain impractical for placement within these intricate technological designs for nanoelectronics, although some have proposed using the very devices themselves for such metrology, negating the need for a target (19). Targets small enough to be placed within the active area of the electronics, also called "indie", require spatial resolution enabled by high-magnification techniques such as microscopy. Commercial efforts to measure such targets have concentrated initially on the measurement of the relative displacement of one photolithographic layer with another, called "overlay offset" and the term applied to these in-die measurements using physical optics is "uDBO" or micro-diffraction-based overlay (20-23).

Prior to the introduction of  $\mu$ DBO, our group proposed and realized what we termed "scatterfield microscopy" (3, 4, 24-26), an approach to microscopy that combines sophisticated illumination engineering with the optimized collection of information from the full 3-D electromagnetic scattered field about targets of interest. Imaging these targets permits spatial localization of a region of interest (ROI) smaller than the scatterometric spot size, and several targets can be imaged within the field of view of the microscope without degrading the dimensional measurements (27). Our group has also yielded image-based measurements of overlay using finite sets of arrayed lines (3) and has also concentrated on the measurement of line width, often referred to in nanoelectronics as the "critical dimension" (CD) (28).

To better manipulate the scattered electromagnetic field, our scatterfield microscope designs feature a plane conjugate to the back focal plane (BFP) of the objective lens (29). Illustrated in Fig. 2 (a), angular control can be realized if one uses a Köhler illumination (30) scheme as shown; blocking light at the BFP defines the angular resolution of the illumination. In our microscopes, we access a conjugate to the BFP (CBFP) within a high-magnification platform. Selected methods for angular control are illustrated in Fig. 2 (b). First, one can use an annulus to define a narrow cone of allowed illumination numerical apertures (INAs). Likewise, slits can be employed to limit the NA differently in orthogonal directions. Recent studies by our group have shown increases sensitivity to CD by tailoring the partial coherence factor and aperture shape in the CBFP (31). Quadrupole and dipole illumination have also been explored for enhancing the optical response from pattered

samples (32, 33). Second, instead of an annulus or slit, a single finite aperture can be used to produce a narrow cone of light at the sample (25). Using two-axis automated stages in the CBFP, this aperture can be scanned to yield goniometric reflectometry. Linear polarizers are often employed close to the CBFP and on occasion have been used on the imaging path. Fig. 2 (c) shows one calibration of the CBFP position as a function of angle of incidence for the NIST Visible-Light Scatterfield Microscope.



Figure 2. Schematic diagrams describing key elements of Scatterfield microscopy. (a) Angularly resolved illumination from Köhler illumination, from (34). (b) Apertures utilized on the NIST 193 nm Microscope, as imaged at a Fourier plane conjugate to the BFP. Left panel shows multiple realizations of  $0^{th}$  order reflection of a single aperture scanned across the CBFP, from (32). Right panel shows a dipole. (c) Angular distribution measurement at the NIST Visible-Light Microscope. Successive images of the illumination are measured as the sample stage is lowered; the measured changes in positions below the sample plane is divided by the *z* movement to derive the tangents of the incident angles of illumination.



Figure 3. Angle scan measurements using scatterfield microscopy, measuring (a) nominally 100 nm wide arrayed cylinders, determined to be conical with an elliptical base ( $\lambda = 450$  nm), with 1 $\sigma$  uncertainties based on repeated experiments. (b) Resist layer on Si ( $\lambda = 193$  nm), from (36), with experimental data uncertainties plotted for a  $2\sigma$  confidence interval.

Figure 3 shows two examples of angle scans, one employing  $\lambda = 450$  nm light at the NIST Visible-Light Scatterfield Microscope (37) and one in the deep-ultraviolet using the NIST 193 nm Microscope (38). The lack of data in Fig. 3 (b) for  $-17^{\circ} < \theta < 17^{\circ}$  is due to the central obscuration in the catadioptric lens utilized on this deep-UV instrument. Initial quantitative measurements by our group concentrated on exploiting this goniometric reflectometry. Similar angle-resolved experiments have been performed by others under the name "microscatterometry" (39, 40). Such angle-scans with fitting have been performed for arrays of Si lines (41), for arrays of nitride lines (37), and for three-dimensional arrays of Si pillars (35).

Quantitative fitting has also been achieved as a function of spatial position for finite features and arrays by using intensities in the *x*-*z* plane (as opposed to the actual image in the *x*-*y* plane). Starting from a single step height in Si, focus-resolved measurements have been carried out with fitting. These results were subsequently augmented with more careful measurements of the optical transmissivity of the physical optics as a function of illumination and collection angle and applied to a nominally 100 nm CD, 600 nm pitch Si line array (34). Aberrations and variations in transmissivity were rectified by altering the simulation data, allowing better fitting between imperfect experimental data and now-imperfect calculation results. In addition, the nature of the correlation among the different noise sources was accounted for and incorporated into the regression. From these combined efforts, our group reported fits between theory and experiment for three separate targets comprised of thirty lines each (42). Feature widths as small as 15 nm, or  $\lambda/30$ , were measured quantitatively. Examples of this comparison for 100-line targets are shown as Fig. 4.



Figure 4. Data fitting of intensity data acquired using scatterfield microscopy at two polarizations and 21 focus positions. After (42).

These examples have shown that much information can be extracted about subwavelength features using a fixed-wavelength, high-magnification platform through polarization control, defined incident angles, multiple focus positions, target design, and materials choices. These assume a foreknowledge of the nominal state of the patterning. We have also thoroughly researched the optical response due to errors in such patterning, called "defect metrology" (43) in nanoelectronics. Scatterfield techniques have been applied to maximize the unresolved optical response as functions of polarization (44), incident angles (33), inspection wavelength (45), and even volumetrically (46) by assessing images at multiple focus heights. Nevertheless, some inherent challenges may persist despite these optimizations, which are addressed in the next section.

# Enhancing Data Processing for Contemporary Nanoelectronics Metrology

# Hybrid Metrology

In the previous section, correlation among parameters was described as a problem that affects angle-resolved scans acutely. While spectroscopic methods may avoid some of these challenges, it is still fundamentally limited by these parametric correlations. As devices grow in complexity especially as emerging materials are further introduced, more parameters than ever will be required to characterize dimensions using scatterometry, increasing the potential for correlations.

In the process of fitting angle-resolved data, our group faced a major challenge due to these correlations, an especially vexing situation as the uncertainty in the height parameter was much larger in optical fitting than from the expanded uncertainty in the height provided by a second NIST instrument, an atomic force microscope. In collaboration with other NIST colleagues, our group sought a methodology that would allow the statistically rigorous incorporation of a second measurement and its uncertainty into our model-based fitting. From this effort, multi-tool measurements with nested uncertainties were introduced to nanoelectronics manufacturing in 2009 (47, 48). The next year, industry built upon the concept and renamed it "hybrid metrology," (49) the accepted name for the technology. Our group and our NIST collaborators have since researched quantitative hybrid metrology (50), hybrid metrology for data with a constant systematic bias (51), and also combined regression, the fitting of two or more model-based measurements simultaneously (52). In response, the industry has published several papers (53-60) often using otherwise "competing" metrology techniques, such as scanning electron microscopy and spectroscopic ellipsometry (60).

# Machine Learning

Another method for dealing with the complexity inherent in current and future dimensional metrology is the application of machine learning. Thus far, our group has concentrated machine learning efforts to improve our defect metrology capabilities (61), but we remain interested in its use for quantitative CD metrology. The use of virtual metrology to analyze scatterometry data has been discussed by some industrial authors (62). One potential downside of such an approach is a disconnect between established physical models of

scattering and the experimental intensity observations. However, recently Schneider *et al.* have published a paper discussing one potential route for performing CD measurements augmented by both machine learning and electromagnetic modeling (63). No matter how the machine learning is performed, if the process control of critical dimensions is enhanced by these new approaches, this aspect of data processing will continue to grow in importance as devices grow in geometric and design complexity.

### **Optics-based Metrology of Emerging Materials**

Due to the speed and non-destructive nature of optical methods, these methods will be required for the process control of novel and advanced computational architectures, especially as emerging materials are integrated into the process flow. How difficult will it be to extend optics-based metrology to these emerging materials? Looking first from an optimistic perspective, optical-methods should be able to accommodate the incorporation of these materials. Optical methods have already advanced well beyond width measurements in the microscale range, progressed into model-based fitting, and have been augmented by measurements from additional technologies through hybrid metrology. Some of the complexity introduced by emerging materials may be mitigated by a precise foreknowledge of its dimensions (e.g., two-dimensional materials). Process control in some cases is already regulated by artificial intelligence, which assesses the optical response but not the underlying physics of the novel material. Even without invoking artificial intelligence, model-based measurements such as optics should continue to function if the optical properties are well characterized for the emerging materials.

A more pessimistic outlook however would question the validity of the assumptions made within the model-based measurements: How do the optical properties of emerging materials differ between those of a free-standing film and those placed within a device? Furthermore, how accurately can even a free-standing film be measured with existing optics-based metrologies? These questions must be addressed without knowing which emerging materials will be best suited for integration into high-volume manufacturing.

As research towards optimal emerging materials advances, many of these same questions can be addressed using conventional complementary metal-oxidesemiconductor (CMOS) materials, including crystalline silicon (c-Si). Our group has recently reported atomistic simulations using density-functional theory (DFT) from which the dielectric function could be determined as a function of film thickness and wavelength (64). The main motivations in the work stem from the potential thickness-dependence of the dielectric function,  $\varepsilon$ , and also its inherent anisotropy. For ultrathin films, a dielectric tensor  $\boldsymbol{\varepsilon}$  is required with in-plane components  $\varepsilon_{xx} = \varepsilon_{yy}$ . Each DFT simulation of hydrogenterminated Si(111) surfaces featured one of seven silicon thickness, from less than 1 nm to more than 6 nm. Results showed  $\varepsilon_{xx}$  converging towards  $\varepsilon_{zz}$  with increasing Si thickness; such relative results should be emphasized as there are various approximations inherent to DFT and involved in obtaining  $\varepsilon = \varepsilon_1 + i \varepsilon_2$  from those DFT results. Goniometric reflectometry simulations of these ultrathin films were reported, with increased systematic bias in the fitting of Si thicknesses  $d_{Si}$  for  $d_{Si} < 6$  nm. Prior information about the thickness greatly improved the fit of both the optical constant k and  $d_{Si}$ , especially if the thickness is known to within 10 %, given the anti-correlation among those parameters.

This study above presupposed a single illumination wavelength, and results will differ for spectroscopic ellipsometry and scatterometry. Furthermore, additional DFT studies and perhaps tight-binding calculations should be performed for the candidate emerging materials. While this might illustrate an optimal candidate material for optics-based metrology, it should be remembered that materials selection in nanoelectronics follows manufacturability and technological requirements, and not the potential for metrological enhancement. Combinatorial methods should be prepared for all possible emerging materials to prepare for their potential integration.

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