OPTICAL CRITICAL DIMENSION METROLOGY
with Spectroscopic Ellipsometry

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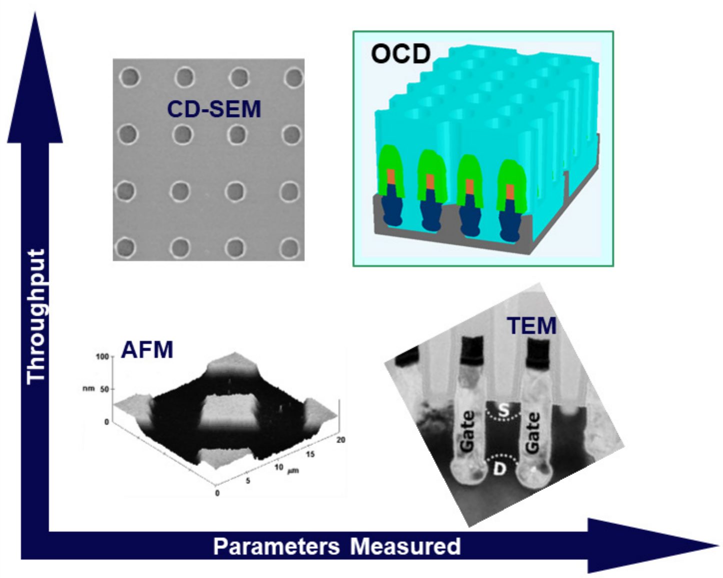


Figure 1. OCD is compared to other CD metrology methods graphed versus throughput and the parameters measured.

Optical critical dimension metrology (OCD), also known as optical scatterometry, has been an integral part of the semiconductor "critical dimension" process control ecosystem for over two decades. OCD has inherent advantages over competing measurement techniques (such as CD-SEM, AFM, and cross-sectional SEM), see Figure 1, because it is non-contact, non-destructive, fast (sub-second acquisition time), and extremely precise. OCD is an indirect, model-based optical technique (typically spectroscopic) that allows for the extraction of critical geometric parameters, asymmetries, and optical properties of periodically patterned structures at sensitivities much less than the measurement wavelength of light (>100x smaller). Such sensitivity to multiple geometric parameters and material properties is due to the use of polarization-sensitive measurement techniques, like spectroscopic ellipsometry, and a sophisticated electromagnetic (EM) solver to simulate the spectral response of a periodic structure. If you already have a spectroscopic ellipsometer, you have the best way to measure thin film thicknesses and optical properties and a potential OCD tool to characterize 3D nanostructures. The missing piece is the analytical modeling software, which is where Ai Diffract©, from Onto Innovation, comes in.

Ai Diffract (or AiD) is a powerful EM modeling and regression engine for OCD metrology with an intuitive 3D modeling interface to simplify building even the most complex structures. Figure 2 shows examples of semiconductor device structures built in the 3D Region Model Editor. AiD is built on over 20 years of development and has been adopted for high-volume production by every major semiconductor manufacturer for process control. In this article, we will provide a brief history of OCD metrology in the semiconductor industry. We provide an overview of the OCD analysis workflow, followed by a brief introduction to model optimization, and then we will show two example use-cases.

A BRIEF HISTORY OF OCD METROLOGY IN THE SEMICONDUCTOR INDUSTRY

The adoption of OCD started in the late 1990s and early 2000s in lithography as a fast way to qualify scanner process windows. This was in reaction to the inability of top-down CDSEMs to determine the bottom critical dimension of photoresist lines when the sidewall angle was greater than 90 degrees (a "reentrant" profile). Early OCD scatterometers were either angle-resolved single wavelength (2-) tools or normal incidence spectroscopic reflectometry tools capable of acquiring "s" and "p" polarization. In contrast, spectroscopic ellipsometry was the workhorse for thin film metrology at that time. This all changed towards the end of the 2000s with the introduction of FinFet devices in advanced logic and the move to 6F2 DRAM in advanced memory. These 3D devices required simultaneous critical dimension and height measurements for optimum process control. However, the model complexity increased by more than double the number of "floating" parameters in the model. Figure 3 compares the relative simplicity of a thin film stack on the left, where the unknown parameters include film thicknesses and possibly material optical constants. In contrast, complex nanostructures can have these same unknowns with the addition of lateral dimensions, as shown in Figure 3 for 2D and 3D devices.

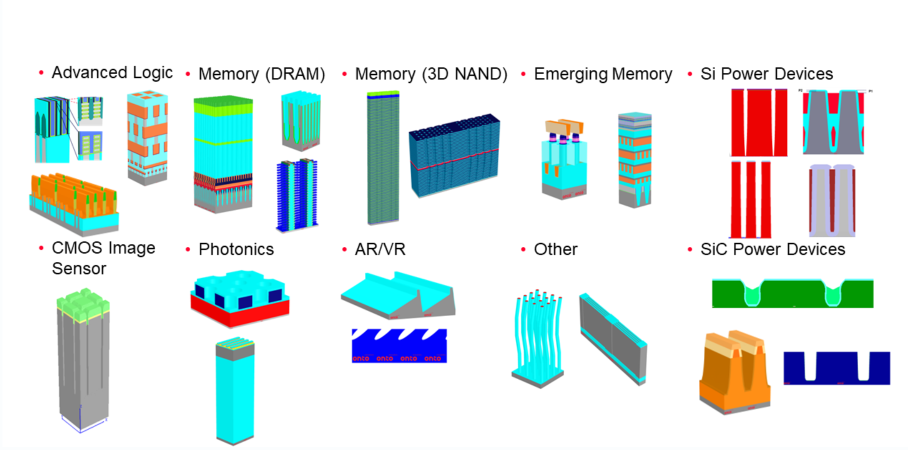


Figure 2. Examples of Semiconductor Devices built in AiD

The increased complexity of 3D structures necessitated spectroscopic ellipsometry and generalized (or Mueller matrix) ellipsometry for OCD to take advantage of their added information content and increased sensitivity. Figure 4 compares the information content from a standard ellipsometry measurement, which assumes an isotropic response from the sample, to the complete response from a Mueller matrix measurement. Instead of the three standard SE data curves (N, C, & S), the Mueller matrix contains 15 normalized data curves accounting for cross-polarization and depolarization effects. The 2010s saw the move to a measurement of on-device structures in logic, like SRAM and electrical test (E-test) devices. This coincides with the introduction of 3D NAND, which further solidified generalized ellipsometry as the standard for raw OCD data. The E-test devices required expanding the spectral range into the infrared.

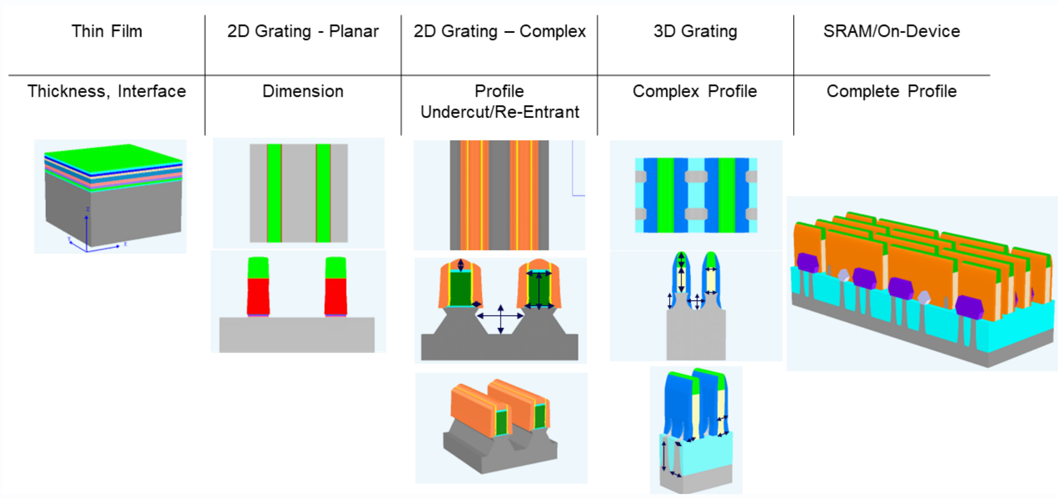


Figure 3. Evolving complexity of Logic devices

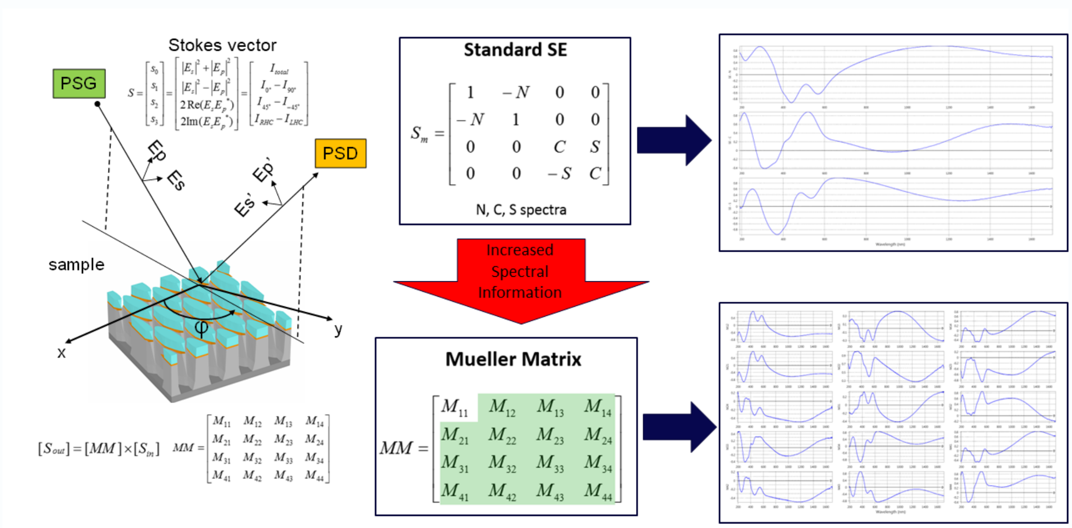


Figure 4. Comparison of "standard" SE and Mueller Matrix SE (MMSE)

THE OCD WORKFLOW

Figure 5 shows the workflow for OCD model creation. In the first step, spectra are acquired on the structure of interest using a spectroscopic ellipsometer. The ellipsometer's azimuth angle relative to the structure (the plane of incidence, POI) is critical to the measurement. There can be optimal POIs for different structures, even for particular geometric parameters in that structure. Breaking the mirror symmetry of a structure with the POI, for example, can be beneficial because it induces a response in the off-diagonal elements of the Mueller matrix, which provides more independent spectral content that can be used to decorrelate parameters (more on this is the next section).

In the second step, the OCD structure is built in AiD using the 3D Region Model Editor. This editor uses a graphical user interface (no need for scripting) and enables the construction of any 3D model using simple building blocks (like trapezoids, columns, fills, spacers, films, and coatings), as demonstrated in Figure 6. The etching functions allow the emulation of a realistic etch process, and the vertical hyper-profiler enables the description of a profile with an N-order orthogonal polynomial.

The third step involves the rigorous coupled-wave analysis (RCWA) based engine, which is the EM solver that outputs a simulated spectrum based on the OCD model and spectral acquisition parameters (like angle of incidence, wavelength range, etc.). RCWA was first developed in the 1980s by Moharam and Gaylord. It starts with the assumption that the structure is periodic and infinite in the lateral dimensions, allowing Maxwell's equations to be rewritten as a Fourier expansion along both X and Y dimensions. In contrast, the Z dimension is separated into slices. The coupled wave equations for every slice in Z are solved using ordinary matrix techniques with matched boundary conditions. Equation 1 and 2 show the expanded Fourier series for electric and magnetic fields and their substitution into Maxwell's equations. Thanks to the wide availability of efficient algorithms for performing Fast Fourier Transforms, this method is computationally efficient and much faster than competing EM solver methods (like FDTD and FDFD). This is an extremely simplified, bordering on absurd, introduction to RCWA, and there are many more rigorous introductions available online, which will be listed at the end of the article.

$$E_{gy} = \sum_i S_{yi}(z)\exp(-jk_{xi}x) \qquad H_{gx} = -j\left(\frac{\varepsilon_0}{\mu_0}\right)^{1/2} \sum_i U_{xi}(z)\exp(-jk_{xi}x)$$

Equation 1. Fourier expansion of E and H fields

$$\frac{\partial S_{yi}}{\partial z} = kU_{xi} \qquad \frac{\partial U_{xi}}{\partial z} = \left(\frac{k_{xi}^2}{k}\right)S_{yi} - k\sum_p \varepsilon_{(i-p)}S_{yp}$$

Equation 2. Maxwell's Equations with the substituted Fourier expansions of E and H fields. S and U are Fourier coefficients of the respective field components.

The fourth step is to compare the measured and calculated spectra from the RCWA engine and then minimize the difference between these two data sets by varying the "floating" parameters. The MSE, or mean squared error, is used as a cost function and totals the difference between the measured and calculated spectra at every wavelength. The floating parameters in the model are defined (like widths, height, sidewall angles, and thicknesses) and then varied non-linearly (using an algorithm like Levenberg-Marquardt) to change the calculated spectrum relative to the experimental measurement until the MSE is minimized to a defined threshold.
Finally, the parameters are reported to a host computer or spreadsheet in the fifth and final step. Floated parameters can be reported, and complete profiles and linear combinations of any parameters can also be reported.

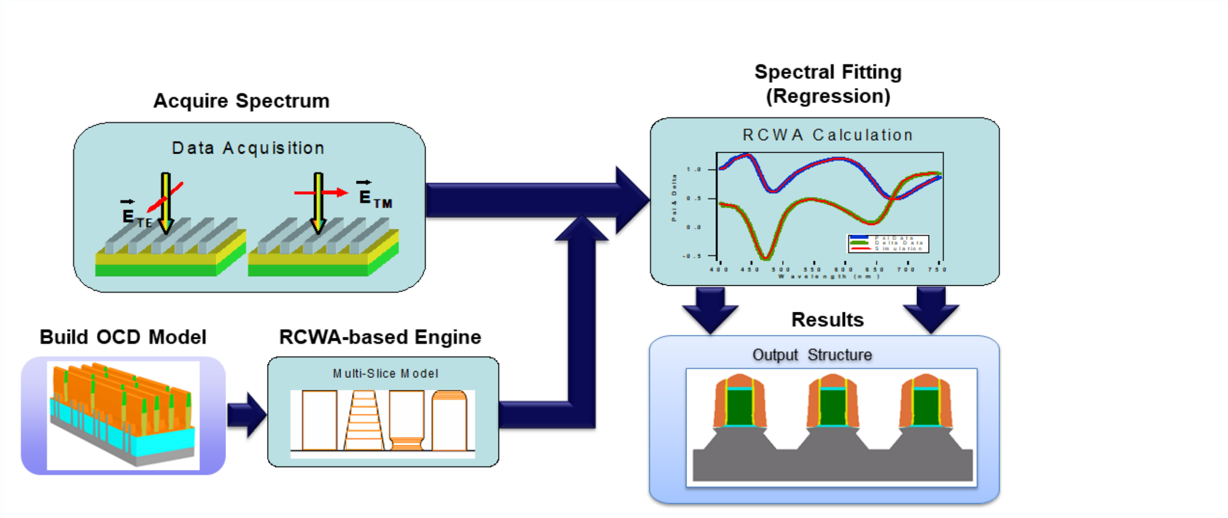


Figure 5. OCD Model Workflow, starting from the left. 1) SE data are acquired. 2) An OCD model is built. 3) An RCWA-based engine calculates the expected response. 4) The unknown sample properties are varied in a spectral fitting process. 5) The results are reported.

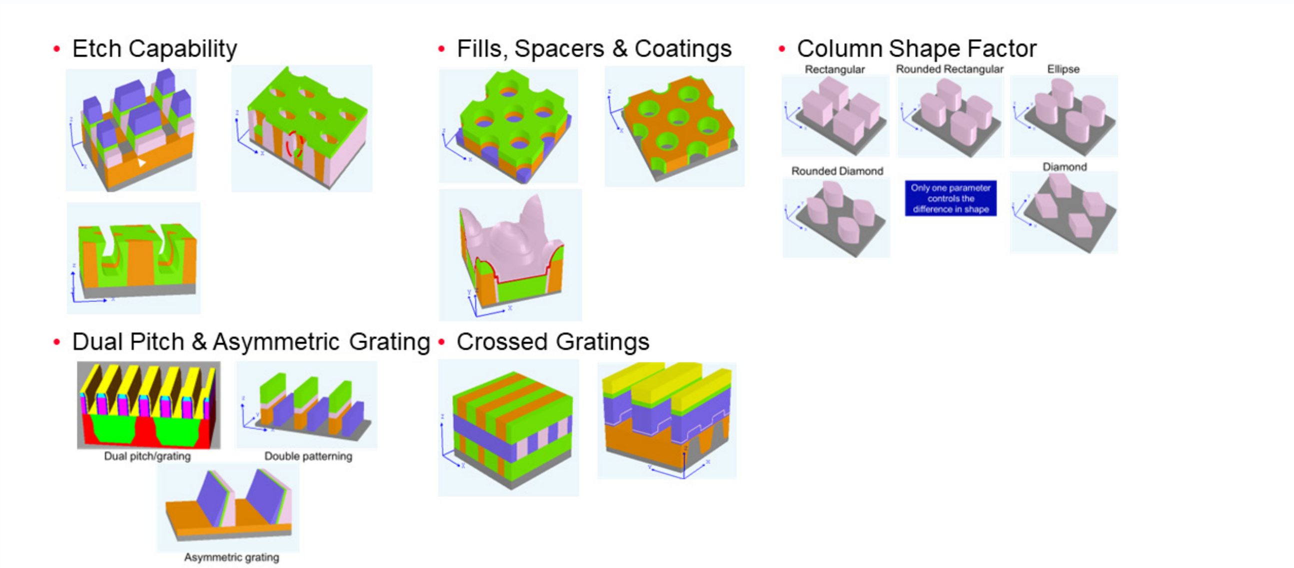


Figure 6. 3D Region Model Capability

OCD MODEL OPTIMIZATION

Like traditional ellipsometry, OCD is an indirect method that requires a model to extract structural parameters. Every "floating" parameter in a model has a sensitivity curve that can be defined as a change in calculated value versus a parameter change. If two or more parameters have similar sensitivity curves in a model, we say that these parameters are correlated. Correlation between parameters is one of the biggest challenges in OCD model development. However, AiD has a built-in tool to optimize the model called "U&SA" (Uncertainty and Sensitivity Analysis). This utility is based on Bayesian analysis, where the inputs are spectral noise (derived from actual measurements and representative of system noise), spectral parameter sensitivity (given by the partial derivative of the spectrum with respect to each floating parameter), and any weighting used in the regression. The output is a probability density function of the parameter uncertainty, given as a standard deviation, as well as the corresponding orthogonal uncertainty, or oSigma (which is essentially parameter uncertainty from the noise alone), degree of correlation (defined as the coefficient of multiple correlations, where the correlation between the given parameter and all other floating (independent) parameters is taken into account) for each parameter, and a 2D parameter correlation matrix. Figure 7 shows the U&SA graphical user interface with all the above features.

An example use-case for U&SA is to find the optimal azimuth angle relative to the major axis of a grating. The structures in Figure 8 are 3D shallow trench isolation (STI) islands in an FCC layout rotated at a 35-degree angle. Four different azimuth angles were simulated using U&SA, and the predicted parameter uncertainty for each parameter in the model was plotted versus the azimuth angle (AZ). Lower values in this bar chart represent improved measurement sensitivity to that critical dimension parameter. The simulation results show that the azimuthal angle significantly affects parameter uncertainty and needs to be optimized.

ANISOTROPIC FLEXIBLE SUBSTRATES

Many flexible polymer substrates exhibit optical anisotropy due to intrinsic or stretch-induced molecular chain orientation such as polyethylene terephthalate (PET), polyethylene naphthalate (PEN), and polyimide. The anisotropy in polymer sheets is typically uniaxial ($n_X = n_Y \neq n_Z$) or biaxial ($n_X \neq n_Y \neq n_Z$). When the transmitted beam is acquired, the index difference creates interference oscillations in the ellipsometry data. This is because the long path length through the sample and the index difference create a phase shift. When there is an in-plane anisotropy ($n_X \neq n_Y$), the ellipsometry data varies depending on the measurement orientation. For anisotropic polymer substrates, generalized or Mueller- matrix spectroscopic ellipsometry data are best suited for measuring cross-polarization between the p- and s- waves. Figure 5 shows our modeling results on a 50-μm-thick PEN substrate from 190 nm to 10 μm. Data analysis in the transparent region utilizes variable angle transmission ellipsometry data where the influence of index differences and sample orientation are evident. An increased number of fit parameters in the absorbing region easily produces high parameter correlations. However, we can break this correlation by analyzing ellipsometry data from several different orientations at the same time. A more detailed description of ellipsometry modeling for various flexible polymer substrates can be found in our publication [3].

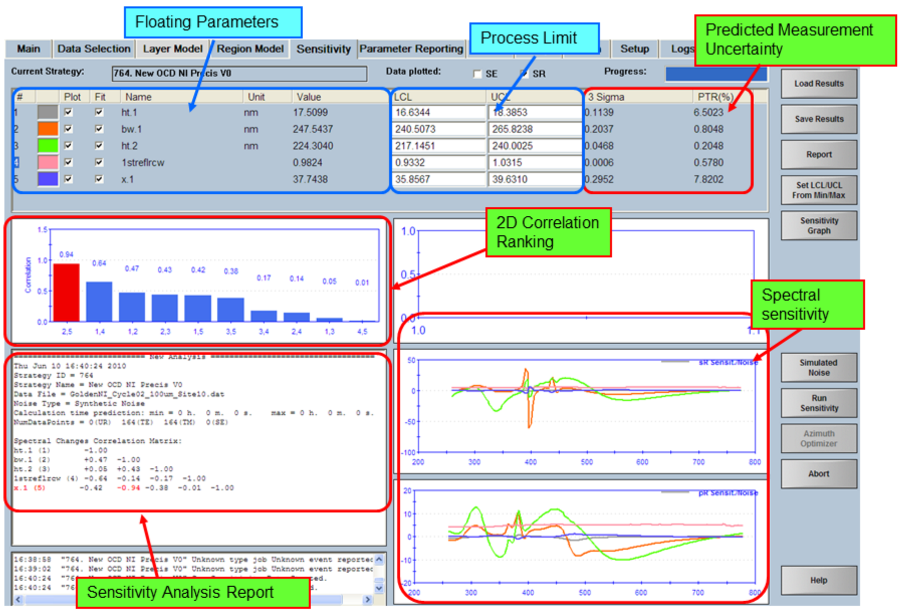


Figure 7. Uncertainty and Sensitivity Analysis graphical user interface in AiD

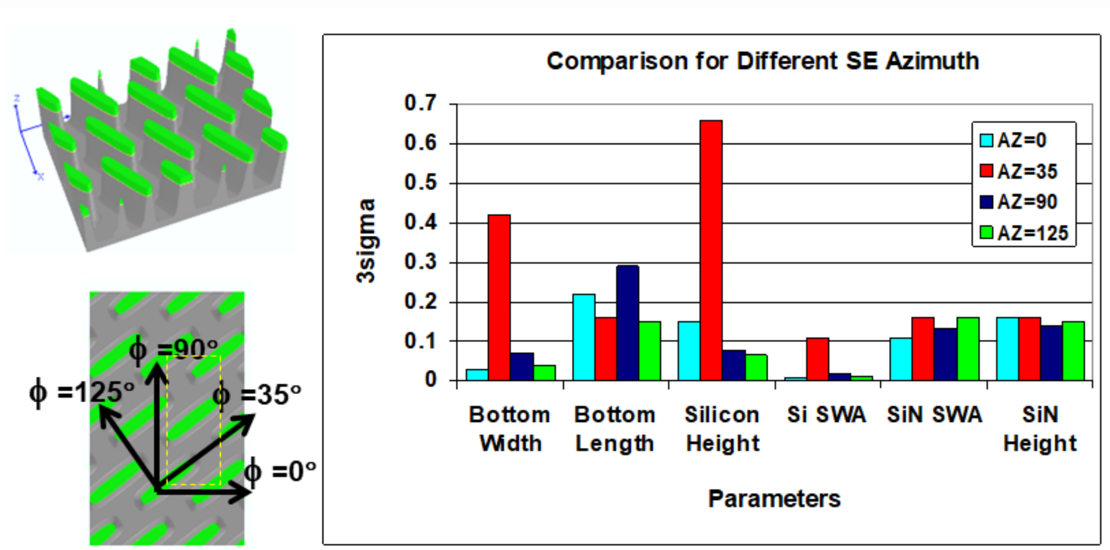
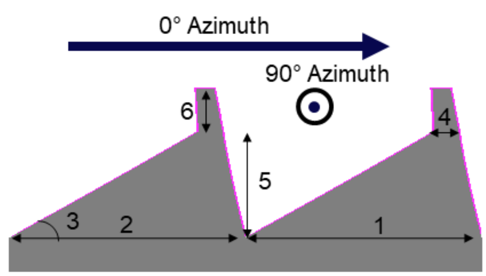


Figure 8. Azimuth Optimization of Rotated STI Island structures using U&SA

EXAMPLE 1: AUGMENTED AND VIRTUAL REALITY (AR/VR) BLAZED GRATING

Surface relief gratings are used in AR/VR applications to couple light into and out of waveguides used in display systems. Slanted gratings are used because they can be tuned to reflect or transmit specific diffraction orders into or out of a waveguide that may be desired for a specific application. In this example, we look at a blazed grating etched into Si, measured at 0 and 90 degrees azimuth angle relative to the grating axis. The free-floating parameters are shown in Figure 9, as are the model fits to the experimental spectra for both POIs. In the 90-degree azimuth orientation, the off-diagonal signal (in the bottom two curves) is a strong function of the asymmetry in the structure from the slanted sidewall, making OCD an excellent technique for characterizing these critical structures in AR/VR applications.



Parameter	Nominal Value
1. Pitch	320-360nm
2. BCD	300-340nm
3. Tilt	40°
4. TCD	30-50nm
5. Si Ht	150nm
6. Si Protrusion	40-60nm

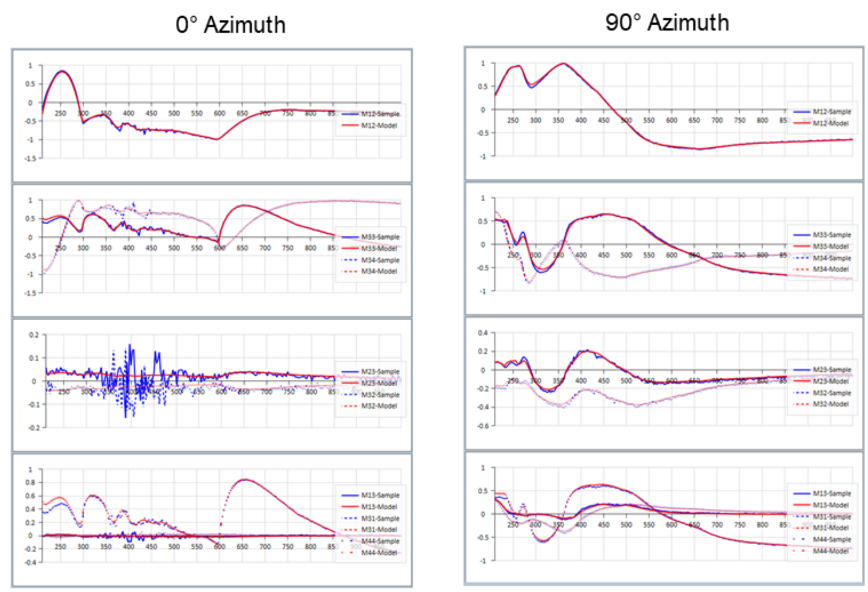


Figure 9. Blazed Surface Relief Grating in Si showing the modeled structure, floating parameters, and model fit at 0 and 90-degree azimuth angles

EXAMPLE 2: SI/SIGE SUPERLATTICE HOLE TEST STRUCTURE

In advanced logic, FinFet transistors have finally "run out of steam" because continued lateral scaling has a negative effect on device performance. All leading-edge logic manufacturers have moved to GAA (gate-all-around) device architectures with "nanosheets" replacing fins as the channel material. To fabricate multiple nanosheets stacked on each other, manufacturers must deposit alternating layers of Si and SiGe, with the SiGe being "sacrificial" in that it will be removed downstream. One of the most critical steps in the process is called "SiGe Cavity Recess Etch," which laterally recesses the SiGe nanosheets relative to the Si nanosheets because it sets the gate length of the device. The Diebold Group at SUNY-Albany has worked on characterizing this step using OCD (and MMSE) and X-ray characterization methods, like XRD and XRF.

The test structure used is an array of elliptical holes at a pitch of 120x240nm. The structure, shown in Figure 10, is four layers of Si/SiGe pairs with a SiN hard mask on top. It is then isotropically etched to create holes and then anisotropically etched to laterally recess the SiGe from the Si. The structure was built in the region model in AiD, and seven floating parameters were defined: Bottom Hole CD Length and Width, Sidewall angle, Silicon over-etch depth, SiN Thickness, Cavity Recess, and Azimuth Angle. Thicknesses of the Si and SiGe were fed forward from thin film (unpatterned) measurements. Figure 11 shows the model fit to the experimental MM-SE spectra acquired at a 75-degree azimuth angle relative to the major axis of the elliptical holes. Figure 12 compares cavity recess measurements from OCD (single and dual azimuth) to transmission electron microscope (TEM) reference measurements. The OCD cavity recess results are less than 0.5nm from the TEM reference values.

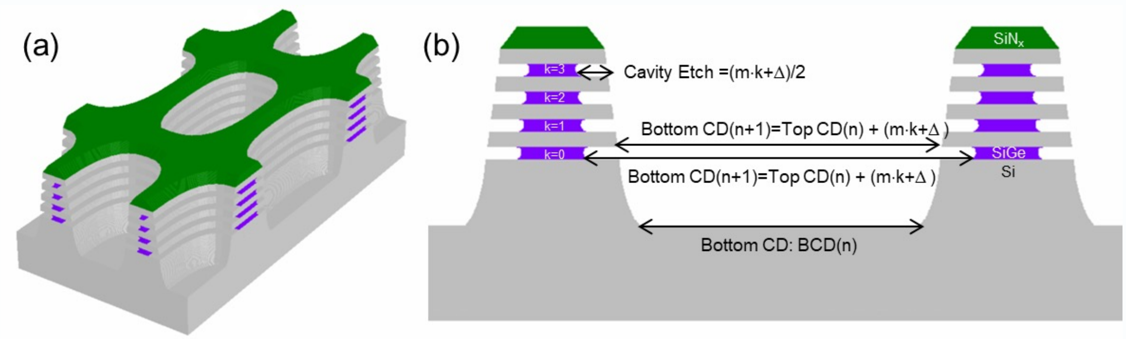


Figure 10. a) Si/SiGe Elliptical Hole Test structure iso view. b) Profile view showing floating CD parameters in the model

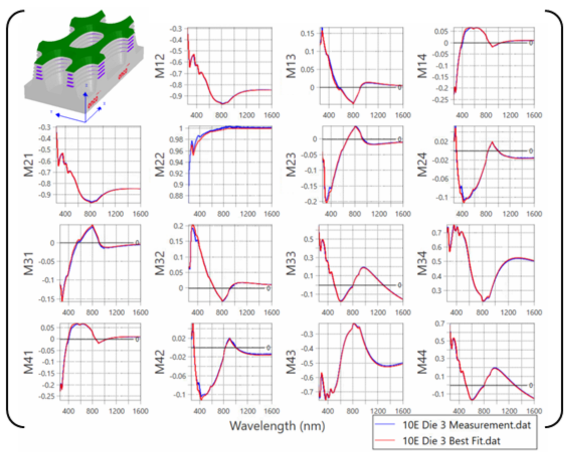
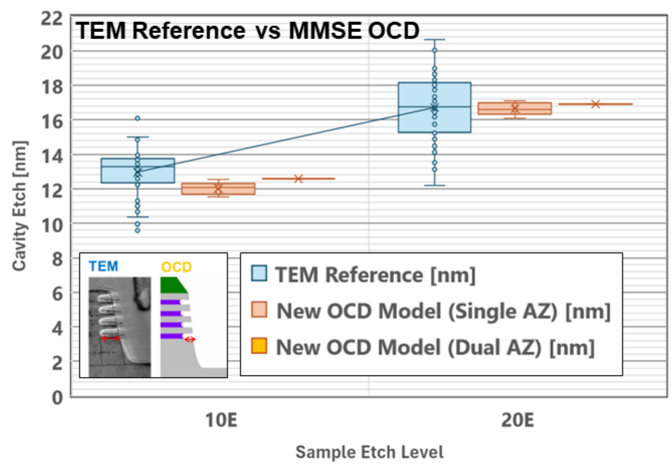


Figure 11. Model fit to Experimental Spectra at 75-degree azimuth angle



Cav Etch Level	TEM Reference [nm]	OCD (Single AZ) [nm]	OCD (Dual AZ) [nm]
10E Avg	13.0	12.0	12.6
20E Avg	16.7	16.6	16.9

CONCLUSION

An introduction to OCD has been presented. We started by comparing competing CD metrology techniques. Then, we went into detail about the history of OCD and its adoption by all major semiconductor manufacturing companies for in-line CD measurements. Next, we went through the workflow of creating an OCD model in AiD and then went through the key built-in optimization tool, U&SA, inside AiD. Finally, we examined two cases where AiD was used for OCD modeling. With its industry-leading spectroscopic ellipsometers, the JA Woollam Company has been a key supplier to Onto Innovation for over 25 years. Now, we would like to open our OCD analysis software to all JA Woollam users so you can turn your ellipsometer into an OCD metrology system!

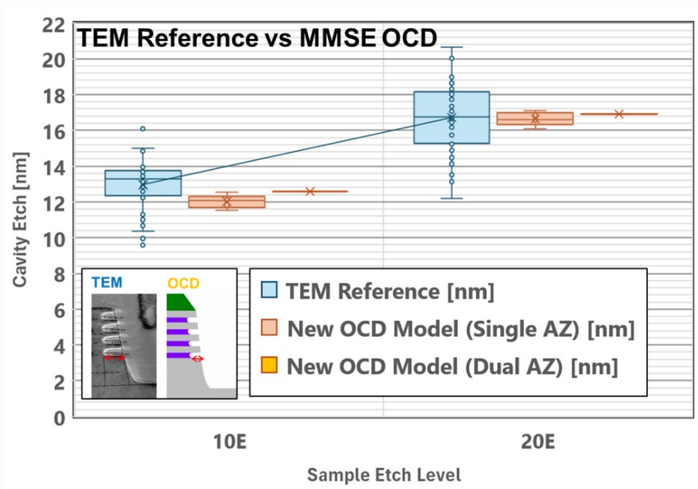


Figure 12. TEM reference vs. OCD results for Cavity Etch

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