Optical Metrology
and Nano Plasmonics

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Nanometrology allows optical inspection of the geometry of nanostructures down to 10nm scale.

It uses a best fit to the measured ellipsometric spectra via theoretical simulation (with efficient software) to determine the critical dimension.

If done correctly, one can reconstruct images of nm resolution by using an optical instrument (with wavelength longer than 100nm).

It is noninvasive and capable of probing buried structures..
Systems of Interest

Metal nanoparticles on a substrate

Nanorods
Buried Self-assembled Quantum Dots

[Shih-Yen Lin (RCAS)]
Outline

◆ Overview of CD Metrology
◆ Rigorous Coupled-Wave Analysis (RCWA)
◆ Green’s function method
◆ Ellipsometric measurements of nanostructures on a substrate & nanorods
◆ SEM studies
◆ Summary
Spectroscopic Ellipsometry

- DUV & visible source
- Polarizer
- Focusing lens
- Wafer
- Compensator
- Collimating lens
- Analyzer
- Detector array
- Diffraction grating
Ellipsometry Basics

1. Known input polarization

2. Reflect off sample ...

3. Measure output polarization

In Jones Matrix representation, ellipsometry measures $\Psi$ and $\Delta$ in:

$$\rho = \tan(\Psi)e^{i\Delta} = \frac{E_{p}^{\text{out}}}{E_{p}^{\text{in}}} = \frac{\tilde{r}_{p}}{r_{p}} = e^{i(\delta_{p} - \delta_{s})}$$
Refractive index

\[ n = \sqrt{\varepsilon} \]

glass window

\[ n = 1.5 \]

Dielectric function

\[ n_1(\lambda) + in_2(\lambda) = \sqrt{\varepsilon_1(\lambda)} + i\varepsilon_2(\lambda) \]

\[ \left( \frac{h c}{\lambda} = \hbar \nu = eV \right) \]
Band structure of GaAs & Dielectric function
Oxide Overlayer Effect (Si)

- Oxide 20Å
- \( \epsilon_{\text{sample}} \)
- \( \epsilon_{\text{overlayer}} \)
- \( \epsilon_{\text{sample}} \)
- \( \epsilon_{1} + i \epsilon_{2} \)
- Si
- SiO\(_{2}\) 20Å
Light is transmitted and reflected or refracted at each interface. Amplitude, phase & polarization are changed by multiple interactions.

Each Attribute (Thickness, Pitch, CD, Profile) Contributes to Unique Ellipsometry Spectral Amplitude of Four Fourier Coefficients, DC, Sin(2ωt), Sin(4ωt), Cos(4ωt) vs Wavelength.
Rigorous Coupled-Wave Analysis

• Most used method for rigorous analysis of optical diffraction by periodic gratings.
• For multilayer system with definite periodicity
• EM fields in each layer are expanded in terms of a finite number (N) of plane waves

\[ E(x,z) = \sum_n C_n(z) \exp\{ik_nx\}; \quad k_n = \frac{2\pi n}{p} \]

• The coefficients \( C_n(z) \) are determined by matching boundary conditions at all interfaces.
• The method is accurate (as long as enough plane waves are used) by not necessarily efficient (scale like \( N^3 \))
A typical fitting to the data of the scatterometry components of $\sin^2\omega$, $\sin^4\omega$, and $\cos^4\omega$. 

![Graph showing fitting to data with wavelength on the x-axis and amplitude on the y-axis. The graph includes DC, Sin2w, Sin4w, and Cos4w labels.]
The RT/CDTM technology combines the standard Opti-Probe® rotating compensator spectroscopic ellipsometer (RCSE) 4 and a high performance (10 GHz) server. RCSE spectra from samples with periodic line/space structures taken on the Opti-Probe® are sent to the server that performs the real-time regression analysis and returns calculated CD profiles as well as underlying film thicknesses.
Application 1
Poly-Si Gate Line at Develop Inspect (DI) Stage

(Data provided by Themawave Inc.)

* This data is wafer dependent. Customer specific data must be gathered with customer wafers.
Application 2

Shallow Trench Isolation

(Data provided by Themawave Inc.)
Evolution of the real time regression fitting from beginning (top figures) to final solution (bottom figures) illustrating how adding feature detail improves the quality of the fit. (Symbols: ●: DC, ▽: Sin(2wt), ■: Sin(4wt), ◊: Cos(4wt)) to measurement results (Lines)
Single \( \{ \text{CD1-4, tPR, tArc} \} \) recipe for monitoring a DI wafer under focus exposure matrix (FEM)
## Comparison of various methods

<table>
<thead>
<tr>
<th>method</th>
<th>complexity</th>
<th>scaling</th>
<th>best for</th>
</tr>
</thead>
<tbody>
<tr>
<td>RCWA (rigorous coupled wave analysis):</td>
<td>1</td>
<td>10(MN^3)</td>
<td>straight grating</td>
</tr>
<tr>
<td>Finite-difference (transfer-matrix method):</td>
<td>1</td>
<td>(MN^3)</td>
<td>any 2D grating</td>
</tr>
<tr>
<td>G0 (multi-layer Green’s function):</td>
<td>3</td>
<td>3KM(N^2)</td>
<td>low contrast 2D/3D</td>
</tr>
<tr>
<td>G1 (ideal grating Green’s function):</td>
<td>5</td>
<td>10N(^3)+5KN(^2)</td>
<td>high contrast 2D/3D</td>
</tr>
<tr>
<td>BIM (boundary-integral method):</td>
<td>8</td>
<td>((2L+fN)(2L)^2)</td>
<td>isolated structure</td>
</tr>
<tr>
<td>BEM (boundary-element method):</td>
<td>10</td>
<td>K(2L+fN)(2L)</td>
<td>isolated structure</td>
</tr>
</tbody>
</table>

N=number of coupled waves  
M=number of slices  
K=number of iterations  
L=number of boundary elements  
f=prefactor for evaluating GF \(\sim 20\)
Green's function method for CD metrology

(a) G0 structure

(b) G1 structure

Numerical procedures

102 Create idealized representation for scatterer.

104 Subdivide perturbation domain into segments.

106 Evaluate wave equation within each segment to create a system of linear equations.

108 Solve linear system to determine the principal-order reflection coefficients for the idealized representation.
Scattering from 2D periodic array of contact holes
Fit to measured data

(sample provided by TSMC)

\[ p = 1000 \text{nm}, \ d = 296.212 \text{nm}, \ t = 409.493 \text{nm} \]
Ellipsometric measurements of Au nanoparticles on a substrate

Motivation

- Au nanoparticles of definite size can be obtained commercially.
- They can be placed on insulating substrate and serve as a mask for making nanostructures.
- It is desirable to have a characterizing tool that can detect the density and uniformity of the distribution of Au nanoparticles on a substrate.
- Ellipsometry is an optical characterizing tool that is noninvasive, can penetrate deep into the material, and can be used in-situ during growth.
- Here we try to explore the capability of ellipsometry for characterizing nanoscale structures on surface or in buried interface.
Nanorods Sample Preparation

(by Gong-Ru Lin, National Taiwan University)

- Developed pattern of Ni particles on oxide on Si
- Transfer oxide pattern
- RIE etching
- Remove oxide and Ni

SEM scan of Si nanorods
Si Nanorods

- G. L. Lin et al., NTU

SEM scan of Si nanorods
Sample Preparation

● APTES (3-aminopropyl triethoxysilane)*
  ■ purity: ≥98.0%
  ■ linear formula: \( H_2N(CH_2)_3Si(OC_2H_5)_3 \)
  ■ formula weight: 221.37
  ■ refractive index: 1.422 @ \( \lambda_0 = 589 \text{ nm} \)

● Sample Preparation Steps:
  ■ silanization: immersed in 1% APTES + 1mM acetic acid for 10 min.
  ■ rinsed with D.I. water and bake at 120ºC for 30 min.
  ■ immersed in aqueous solution with Au nanoparticles for 2 hours.
  ■ rinsed with D.I. water and dried with \( N_2 \) gas.

* http://www.sigmaaldrich.com/catalog/search/ProductDetail/FLUKA/09324
SEM of Au Nanoparticles of different sizes

d = 20nm

d = 60nm

d = 40nm

d = 80nm
VUV-VASE Specifications
(J. A. Woollam Co.)

- Rotating analyzer ellipsometer configuration (RAE) with the addition of AutoRetarder
- Dry nitrogen purge to eliminate absorption from ambient water vapor and oxygen
- Spectral range: 140nm ~ 1700nm
- Angle of incidence: 10° ~ 90°
Ellipsometry Results – Au NP@60°

![Graph showing ellipsometry results for Au NPs at 60° angle of incidence.](image)

- Left graph: Plots of Ψ (degree) versus photon energy (eV) for Au NPs of different diameters (10 nm, 20 nm, 40 nm, 60 nm, 80 nm).
- Right graph: Plots of Δ (degree) versus photon energy (eV) for Au NPs of different diameters (10 nm, 20 nm, 40 nm, 60 nm, 80 nm).

These graphs illustrate the changes in ellipsometric angles as a function of photon energy for Au NPs of varying sizes.
Model fits

- Here we assume Au nanoparticles are sphere like (with diameter d) and placed uniformly on a square lattice with pitch p. The spheres are modeled by 5 to 15 slices of discs.
- We use fixed optical dielectric constants of bulk Au and substrate.
- d=20, 40, 60, 80 nm
- Pitch varies between 40nm-1000nm
- Square lattice + hexagonal lattice
- Calculations performed by GF & RCWA methods
Optical Constants of Gold

source: Ioffe Institute (http://www.ioffe.ru/SVA/NSM/nk/),
data from E. D. Palik, Handbook of Optical Constants of Solids
Models Fitting

- Au nanoparticles (20 nm), angle of incidence: 60°, 65°

Pitch = 80 nm
Model Fitting

- Au nanoparticles (40 nm), angle of incidence: 60°, 65°

Pitch = 160 nm
Model Fitting

- Au nanoparticles (60 nm), angle of incidence: 60°, 65°
- Pitch = 200 nm
Model Fitting

- Au nanoparticles (80 nm), angle of incidence: 60°, 65°

Pitch = 300 nm
Ellipsometry Measurement vs. simulation

- Au nanoparticles: 20, 40, 60, 80 nm
- angle of incidence: 60°
Ellipsometric measurement vs. simulation

- Au nanoparticles: 20, 40, 60, 80 nm
- angle of incidence: 60°
Ellipsometric measurement vs. simulation

- Au nanoparticles: 20, 40, 60, 80 nm
- angle of incidence: 55°
Ellipsometric measurement vs. simulation

- Au nanoparticles: 20, 40, 60, 80 nm
- angle of incidence: 55°
Ellipsometric Measurement vs. simulation

- Au nanoparticles: 20, 40, 60, 80 nm
- Angle of incidence: 65°


Ellipsometric Measurement vs. simulation

- Au nanoparticles: 20, 40, 60, 80 nm
- angle of incidence: 65°
Near-field enhanced imaging ellipsometer
Summary

● Samples with different sizes of Gold nanoparticles immobilized on a glass substrate are investigated by variable-angle spectroscopic ellipsometry (VASE) in the UV to near IR region.
● Both the Green’s function method and rigorous coupled-wave analysis (RCWA) were used to model the ellipsometric spectra.
● GF method is 10 – 100 times more efficient than RCWA in most cases.
● Our model calculations show reasonable agreement with the ellipsometric measurements.
● This demonstrates that the spectroscopic ellipsometry could be a useful tool to provide information about the size and density of nanoparticles deposited on insulating substrate.
● The technique can be extended to inspect buried nanostructures.
Plasmonic Infrared emitter
[Optics Exp. 15, 14673 (2007)]
Angle-dependent reflectance spectra

$L=3000\text{nm}, fL=1900\text{nm}, t_g=100\text{nm}, t_w=25\text{nm}$
Relation between the reflection and emission

\[ Emission(\lambda) = TR(\lambda) \left( 1 - \int_0^{\pi/2} R(\lambda, \theta) \cos(\theta) d\theta \right) \]

For a low loss material, (1-R)~absorption

Each resonant mode in the reflectance spectrum corresponds to an emission peak.

Kirchhoff's law

260°C simulation
220°C simulation
220°C measurement
260°C measurement
Summary

• IR emitter made of plasmonic multilayer structure was investigated experimentally and theoretically.
• The grating-coupled and localized SPP modes were identified.
• Multiple LSPP peaks of the metal/dielectric/metal cavity are suppressed in the T-gate structure.
• The angular dependent reflectance spectrum of T-gate array shows a clear resonant dip, whose wavelength can be tuned by the permittivity of the filler material.
• Using Kirchhoff’s law, the thermal radiation of the proposed structure shows a sharp peak at 3.5 mm with low sideband emission.
• This narrow bandwidth emission is very useful for studies of reactions of biological systems, environmental surveillance, and other industrial applications.