Spectral ellipsometry of periodic nanostructures

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Outline

- CWM - theoretical approach
- Experimental arrangement of spectral ellipsometry
- Applied gratings
- Experimental and theoretical results
- Conclusions
Coupled Wave Method (CWM) implemented as Fourier Modal Method (FMM) can be used to describe the propagation of electromagnetic field in periodical structures. The combination of spectral ellipsometry and CWM has been applied to specify the optical and geometrical parameters of gratings.
Coupled Wave Method

geometry

\[ \lambda \theta (x,y) \]

\[ \nu = 1, 2, \ldots, (K-1), K \]

\[ h^{(k)} \]

substrate
The dimensionless Cartesian position vector is introduced:

\[ x = (x_1, x_2, x_3) = k_0(x, y, z) \]

The time dependence by the factor \( \exp(i\omega t) \) is assumed but formally suppressed.
Coupled Wave Method (CWM)

Governing Maxwell system in the \(\nu\)-th layer

\[
\nabla \times \mathbf{H}^{(\nu)} = \imath \varepsilon^{(\nu)} \mathbf{E}^{(\nu)} ,
\nabla \times \mathbf{E}^{(\nu)} = -\imath \mathbf{H}^{(\nu)}
\]

(free space values \(Z_0 = \sqrt{\mu_0 / \varepsilon_0}\) incorporated in the field \(\mathbf{H}\))

Boundary conditions: \(E^{(\nu)}_j = E^{(\nu+1)}_j , \quad H^{(\nu)}_j = H^{(\nu+1)}_j , \quad j = 1, 2\)

A representation of field components and material functions by two-fold Fourier expansion is the basic principle of Fourier Modal Method (FMM).
Coupled Wave Method (CWM)

Field components expansion (Fourier series)

\[
E^{(v)}_{jm} = \sum_{q} \sum_{m} \sum_{n} u^{(v)}_{jm} e^{(v)}_{q} \exp\{-i(\alpha_{m} x + \beta_{n} x + \gamma_{q}^{(v)} x^{3})\}
\]

\[
H^{(v)}_{jm} = \sum_{q} \sum_{m} \sum_{n} u^{(v)}_{jm} h^{(v)}_{q} \exp\{-i(\alpha_{m} x + \beta_{n} x + \gamma_{q}^{(v)} x^{3})\}
\]

\[
\alpha_{m} = n^{(0)} \sin \phi \sin \varphi + \lambda_{m} / \Lambda_{x}, \quad \beta_{n} = n^{(0)} \cos \phi \sin \varphi + \lambda_{n} / \Lambda_{y}, \quad m, n \in \mathbb{Z}
\]

\[
\varepsilon^{(v)}_{ij} = \sum_{k} \sum_{l} c^{(v)}_{ij} \exp\{-i(\lambda_{k} x_{1} / \Lambda_{x} + \lambda_{l} x_{2} / \Lambda_{y})\}
\]
Coupled Wave Method (CWM)

Rearranged Maxwell system (layer index omitted)

\[-\beta_n h_{3mn} + \gamma h_{2mn} = \sum_{j=1}^{3} \sum_{k=1}^{3} \sum_{l=1}^{3} c_{1j,m-k,n-l} e_{jkl}\]

\[-\gamma h_{1mn} + \alpha_m h_{3mn} = \sum_{j=1}^{3} \sum_{k=1}^{3} \sum_{l=1}^{3} c_{2j,m-k,n-l} e_{jkl}\]

\[-\alpha_m h_{2mn} + \beta_n h_{1mn} = \sum_{j=1}^{3} \sum_{k=1}^{3} \sum_{l=1}^{3} c_{3j,m-k,n-l} e_{jkl}\]

\[
\begin{align*}
\beta_n e_{3mn} - \gamma e_{2mn} &= h_{1mn} \\
\gamma e_{1mn} - \alpha_m e_{3mn} &= h_{2mn} \\
\alpha_m e_{2mn} - \beta_n e_{1mn} &= h_{3mn}
\end{align*}
\]
**Coupled Wave Method (CWM)**

**Eigenvalue problem**

Rearranged Maxwell system solved as eigenvalue problem by finite truncation of Fourier spectra gives eigenvectors $g_q = (e_{1q}, h_{2q}, e_{2q}, h_{1q})$ and eigenvalues $\gamma_q$.

Column vectors of Fourier coefficients are specified as following

$$e_j = (e_{j,-M,-N}, \ldots, e_{j,-M,N}, e_{j,-M+1,-N}, \ldots, e_{j,-M+1,N}, \ldots, e_{j,-M,N}, \ldots, e_{j,M,N})^T$$

Structured matrix of eigenvectors

$$D = (g_q) = \begin{bmatrix}
[e_{1q}^+ s] & [e_{1q}^+ p] & [e_{1q}^- s] & [e_{1q}^- p] \\
[h_{2q}^+ s] & [h_{2q}^+ p] & [h_{2q}^- s] & [h_{2q}^- p] \\
e_{2q}^+ s & e_{2q}^+ p & e_{2q}^- s & e_{2q}^- p \\
h_{1q}^+ s & h_{1q}^+ p & h_{1q}^- s & h_{1q}^- p
\end{bmatrix}$$
**Coupled Wave Method (CWM)**

Wave coupling

**Wave coupling in multilayer**

(v) - th layer attributes:

- amplitude coefficients $u^{(v)}$ ($4d$ – dimensional vector, $d = (2m_{max}+1)(2n_{max}+1)$)
- propagation matrix $P^{(v)}(x_3) = \text{diag}(\exp\{-i\gamma^{(v)}_q x_3\})$, $\gamma^{(v)}_q$ eigenvalues
- matrix of eigenvectors $D^{(v)}$

**Boundary conditions** at interface interface $\zeta^{(v)} = k_0(h^{(1)} + \ldots + h^{(v)})$ between (v–1)-th and v-th layer:

$$D^{(v-1)} \cdot P^{(v-1)}(\zeta^{(v)}) \cdot u^{(v-1)} = D^{(v)} \cdot P^{(v)}(\zeta^{(v)}) \cdot u^{(v)}$$
Coupled Wave Method (CWM)

Total matrix of system

Coupling in multilayer

\[
\begin{align*}
\mathbf{u}^{(0)} &= \mathbf{M} \cdot \mathbf{u}^{(K+1)}, \\
\mathbf{M} &= \left(\mathbf{D}^{(0)}\right)^{-1} \cdot \prod_{v=1}^{K} \mathbf{S}^{(v)} \cdot \mathbf{D}^{(K+1)} \\
\mathbf{S}^{(v)} &= \mathbf{D}^{(v)} \cdot \mathbf{P}^{(v)} (-k_0 h^{(v)}) \cdot \left(\mathbf{D}^{(v)}\right)^{-1} \ldots \text{contribution of the } v\text{-th layer}
\end{align*}
\]

structured for reflection \((\mathbf{u}^{(0)-})\) and transmission \((\mathbf{u}^{(K+1)+})\) coefficients:

\[
\begin{bmatrix}
\mathbf{u}_s^{(0)+} \\
\mathbf{u}_s^{(0)-} \\
\mathbf{u}_{ss}^{(0)+} \\
\mathbf{u}_{sp}^{(0)+}
\end{bmatrix} = \mathbf{M} \cdot
\begin{bmatrix}
\mathbf{0} \\
\mathbf{u}_s^{(K+1)+} \\
\mathbf{u}_{ss}^{(K+1)+} \\
\mathbf{u}_{sp}^{(K+1)+}
\end{bmatrix}
\quad \text{or} \quad
\begin{bmatrix}
\mathbf{0} \\
\mathbf{u}_p^{(0)+} \\
\mathbf{u}_{ps}^{(0)+} \\
\mathbf{u}_{pp}^{(0)+}
\end{bmatrix} = \mathbf{M} \cdot
\begin{bmatrix}
\mathbf{u}_{ps}^{(K+1)+} \\
\mathbf{u}_{pp}^{(K+1)+}
\end{bmatrix}
\]
Coupled Wave Method (CWM)

Ellipsometric angles

Reflection properties of the measured samples are described by complex ellipsometric ratio \( \rho(0) \) (we assume that the incident light is linearly polarized at azimuth \( \theta = \pi/4 \))

\[
\rho(Q(0)) = \frac{u(pp,Q(0)) -}{u(ss,Q(0)) -}
\]

where \( Q = 1, \ldots, 4d, \ d = (2m_{max}+1)(2n_{max}+1) \). The sign “-“ respects the negative direction considering \( z \)-axis.
Experimental arrangement

computer controlled four zone null ellipsometer with polarizer-sample-compensator-analyzer (PSCA) configuration in the spectral region from 240 to 700 nanometers
Applied gratings

- Si$_3$N$_4$/SiO$_2$/Si binary gratings
- SiO$_2$ lamellar gratings
- Si lamellar gratings
- Ta lamellar grating and paraboloidal wires
Results

$Si_3N_4/ SiO_2/ Si$ binary gratings

- $Si_3N_4/SiO_2/Si$ binary gratings
- 100 x 100 μm
- periodicity 250 μm
- thickness cca 220 nm
Results

Si$_3$N$_4$/ SiO$_2$/ Si binary gratings

All measurements in this case have been performed at the geometrical configuration when the plane of incident light was parallel to dot edges.
Results

Si$_3$N$_4$/ SiO$_2$/ Si binary gratings

The dispersion properties have been computed following refractive indices of silicon substrate and Si$_3$N$_4$ dots from Palik.

The relevant parameters for SiO$_2$

\[ \varepsilon(\lambda) = 1 + A\lambda^2 (\lambda^2 - B^2)^{-1} \]

where

A = 1.1336 and B = 92.61 nm.
Results

Si$_3$N$_4$/ SiO$_2$/ Si binary gratings

- The shifts of ellipsometric angles generated by this oxidation process have been computed for planar structures and parallely confirmed by experiment on SiO$_2$/Si. The oxidation process decreases $\Delta$ parameters; for values of $\psi$ we can observe the opposite tendency.
Results

Si$_3$N$_4$/ SiO$_2$/ Si binary gratings

Plane of incidence is in the first case parallel with dot edges; in the second one this configuration has been oriented diagonally.
Results

Si$_3$N$_4$/ SiO$_2$/ Si binary gratings

**Incidence angle**
In the frame of $\Delta$ parameters we can observe the differences higher than 10 degrees if the change of incidence angle is 2 degrees. The main feature of $\varphi_i$ influence is the decreasing of ellipsometric angles $\Delta$ and $\psi$ for increasing value of $\varphi_i$. This tendency indicates that the measurements were realized at the incidence angles less than “pseudo” Brewster angle.

**Geometrical position of incidence plane**
The differences of relevant values have been analyzed to be less than 0.2 degree for $\psi$ parameters.

**Ultrathin oxidation layer**
The results show the degreasing about 3 degrees for $\Delta$ per one nm of thin film oxidation growth; $\psi$ angles indicate opposite three times less tendency in comparison with $\Delta$ dependency.

**Dot thickness**
The computed curves for the dispersion of these angles predict that the thickness accuracy about 3% can be arrived.

**Refractive index dispersion**
Relatively small changes in refractive index dispersion of dots create important amplitude and resonant shifts in ellipsometric angles distribution as function of wavelength.
Lamellar gratings

Airy-like internal reflection series (AIRS)

\[ f'^r = \sum_{j=0}^{\infty} f'_j \]

\[ f' = R^{01} f^l \]

\[ f'^l = T^{12} P^1 T^{01} f^l \]

\[ f^l = \sum_{j=1}^{\infty} f^j \]
Results

SiO$_2$ lamellar gratings

$\Lambda = 260$ nm, $W = \Lambda - \Delta = 80, 100, 130, 150, 180$ nm (A, B, C, D, E)

$d = 525$ nm, $\lambda \epsilon (270, 700)$

$\epsilon (\lambda) = 1 + \frac{A \lambda^2}{\lambda^2 - B^2}$, $A = 1.1336$ and $B = 92.61$ nm
Results

SiO$_2$ lamellar gratings

![Graph showing wavelength vs. angle (Ψ) and measured values for different n$_{max}$ values.]

<table>
<thead>
<tr>
<th>$n_{max}$</th>
<th>1</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d$</td>
<td>498.18</td>
<td>503.86</td>
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<tr>
<td>$W$</td>
<td>102.82</td>
<td>100.64</td>
</tr>
<tr>
<td>$\Lambda$</td>
<td>257.84</td>
<td>257.91</td>
</tr>
<tr>
<td>error</td>
<td>3.34</td>
<td>3.42</td>
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</table>
Results
Si lamellar grating

\[ \psi \] [deg]

\[ 0.4 \quad 0.5 \quad 0.6 \quad 0.7 \quad 0.8 \quad 0.9 \]

Wavelength [nm]

\[ 300 \quad 400 \quad 500 \quad 600 \quad 700 \quad 800 \]

\[ n_{\text{max}} = 2 \]
\[ n_{\text{max}} = 10 \]

<table>
<thead>
<tr>
<th>( n_{\text{max}} )</th>
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<th>10</th>
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<tbody>
<tr>
<td>( d )</td>
<td>116.00</td>
<td>116.71</td>
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<tr>
<td>( W )</td>
<td>49.16</td>
<td>47.07</td>
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<tr>
<td>( \Lambda )</td>
<td>137.09</td>
<td>134.11</td>
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<tr>
<td>error</td>
<td>2.54</td>
<td>2.70</td>
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</table>
Results

Ta lamellar grating

<table>
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<th>4</th>
<th>10</th>
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<tr>
<td>d</td>
<td>248.87</td>
<td>250.11</td>
<td>249.60</td>
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<tr>
<td>W</td>
<td>75.63</td>
<td>78.83</td>
<td>82.64</td>
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<tr>
<td>$\Lambda$</td>
<td>182.78</td>
<td>190.15</td>
<td>189.84</td>
</tr>
<tr>
<td>error</td>
<td>9.02</td>
<td>9.93</td>
<td>10.35</td>
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</table>
Results
Ta paraboloidal grating ($n_{\text{max}} = 20$)

<table>
<thead>
<tr>
<th>$N$</th>
<th>$d$</th>
<th>$W_{\text{max}}$</th>
<th>$W_{\text{top}}$</th>
<th>$\Lambda$</th>
<th>error</th>
</tr>
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<tbody>
<tr>
<td>3</td>
<td>231.60</td>
<td>96.48</td>
<td>60.85</td>
<td>194.63</td>
<td>8.33</td>
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<tr>
<td>5</td>
<td>226.29</td>
<td>99.06</td>
<td>55.81</td>
<td>197.63</td>
<td>5.19</td>
</tr>
<tr>
<td>10</td>
<td>222.37</td>
<td>101.37</td>
<td>53.20</td>
<td>198.41</td>
<td>4.07</td>
</tr>
<tr>
<td>20</td>
<td>219.27</td>
<td>103.79</td>
<td>49.41</td>
<td>199.20</td>
<td>4.01</td>
</tr>
</tbody>
</table>
Results

Ta paraboloidal grating (N = 20)
Results

Convergence properties

SiO₂ rectangular

Si rectangular

Ta rectangular

Ta sliced (N = 3)

Ta sliced (N = 20)

Ta sliced (n_max = 20)
Conclusions

- Rectangular-relief grating of arbitrary depth can be correctly evaluated without slicing, which makes the method highly efficient.

- Comparing the convergence properties according to increasing $n_{\text{max}}$ and $N$, we may conclude that all transparent, semiconductor and metallic gratings can be numerically analyzed with surprisingly good computer time & memory efficiency.

- Semiconductor and metallic gratings with longer periods (compared to the wavelength) require longer-time calculations.