Overview of Optical Metrology of Advanced Semiconductor Materials

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Linear Optical Response of Materials
Spectroscopic Ellipsometry
Advanced Materials in the Semiconductor Industry
Photoreflectance
Photoluminescence
Conclusions
Acknowledgements
Linear Optical Response of Materials

(a) Intraband Absorptions
(b) Phonon Absorptions
(c) Molecular Bond Vibrations

Intraband Absorptions
Interband Absorptions
Phonon Absorptions
Electronic Transitions
Molecular Bond Vibrations
Bandgap

Metals
Semiconductors
Dielectrics
Spectroscopic Ellipsometry: Light polarized in plane of reflection reflects differently than light polarized perpendicular to plane of reflection.

Fresnel Reflection Coefficients different for S and P polarizations

\[ r_{12}^P = \frac{N_2 \cos \phi - N_1 \cos \phi'}{N_2 \cos \phi + N_1 \cos \phi'} \]
\[ r_{12}^S = \frac{N_1 \cos \phi - N_2 \cos \phi'}{N_2 \cos \phi + N_1 \cos \phi'} \]

\[ R^P = \frac{r_{12}^P + r_{23}^P e^{-i2\beta}}{1 + r_{12}^P r_{23}^P e^{-i2\beta}} \]
\[ R^S = \frac{r_{12}^S + r_{23}^S e^{-i2\beta}}{1 + r_{12}^S r_{23}^S e^{-i2\beta}} \]

\[ \tan \Psi e^{i\Delta} = \frac{R^P}{R^S} \]
\[ \Psi = \tan^{-1}\left( \frac{R^P}{R^S} \right), \Delta = \delta_i - \delta_r \]

P designation used for light polarized in plane of reflection (parallel)
S designation for light perpendicular to plane of reflection (senkrecht)
Spectroscopic Ellipsometry

Optical Model

Regression

Thickness and optical properties

\[ \tilde{\varepsilon} = \varepsilon_1 + i\varepsilon_2 = (\tilde{N})^2 = (n + ik)^2 = (n^2 - k^2) + 2ink \]

\[ \alpha = \frac{4\pi k}{\lambda} \]

---

**Refractive Index**
- **Bulk Si**
- \( n \)
- \( k \)

**Dielectric Function**
- **Bulk Si**
- \( \varepsilon_1 \)
- \( \varepsilon_2 \)

**Absorption Coefficient**
- **Bulk Si**
- \( \alpha \)

\( \Psi \) - amplitude ratio, \( \Delta \) - phase difference, \( R \) - Fresnel reflection coefficient, \( n \) - real part of the refractive index, \( k \) - extinction coefficient, \( \varepsilon_1 \) - real part of the dielectric function, \( \varepsilon_2 \) - imaginary part of the dielectric function, \( \alpha \) - absorption coefficient, \( \lambda \) - wavelength of light.
Linear Optical Response of Materials

- **Intraband Absorptions**
- **Interband Absorptions**
- **Drude**
- **Lorentzian**

- **Phonon Absorptions**
- **Electronic Transitions**

- **Molecular Bond Vibrations**
- **Bandgap**

**Metals**

**Semiconductors**

**Dielectrics**
Optical Metrology of thin metal films (Ni, NiSi, TiN and W)

SE Methods & Limitations

\[ \frac{r_p}{r_s} = (\tan \psi)e^{i\Delta} \quad \Psi \& \Delta \rightarrow n, k \& t \]

- Interference enhancements measurements (angle)
- Transmission intensity
- *In situ* measurements
- Optical constant parameterization

\[ \bar{n} = n - ik \quad \text{Kramers-Kronig Consistency} \]

\[ \varepsilon_1 + i\varepsilon_2 = (n - ik)^2 \]

- Transparent
- Semi-absorbing film
- Absorbing

\[ n = \varepsilon + ik \]

\[ \frac{\varepsilon_1}{\varepsilon_2} = n - ik \]

\[ \frac{\varepsilon_1}{\varepsilon_2} = n + ik \]

\[ \frac{\varepsilon_1}{\varepsilon_2} = n - ik \]

\[ \frac{\varepsilon_1}{\varepsilon_2} = n + ik \]

\[ \varepsilon_1 + i\varepsilon_2 = (n - ik)^2 \]
Drude Oscillator - Free Electron

\[ E = \hbar \omega \]

Lorentz Oscillator - Bound Electron

\[ E = \hbar \omega \]

\[ \varepsilon_1 = \varepsilon_1^f + \varepsilon_1^b \]

\[ \varepsilon_2 = \varepsilon_2^f + \varepsilon_2^b \]
Optical model for metals

\[ \varepsilon_1 = \varepsilon_\infty + \omega_{pb}^2 \frac{\tau_b^2 (\omega_o^2 - \omega^2)}{\tau_b^2 (\omega_o^2 - \omega^2)^2 + \omega^2} - \omega_{pf}^2 \frac{\tau_f^2}{\tau_f^2 \omega^2 + 1} \]

\[ \varepsilon_2 = \varepsilon_\infty + \omega_{pb}^2 \frac{\tau_b \omega}{\tau_b^2 (\omega_o^2 - \omega^2)^2 + \omega^2} + \omega_{pf}^2 \frac{\tau_f}{\omega (\tau_f^2 \omega^2 + 1)} \]

From Ellipsometry you can extract \( \tau_f \)

Mayadas and Shatzkes -

\[ \frac{1}{\tau_f} = \frac{1}{\tau_{bulk}} + \frac{\nu_F}{\lambda} \]

\[ \lambda = \left[ \frac{2(1 - \Re)}{3\Re} \right] R_g \]

Mayadas and Shatzkes

\[ \frac{1}{\tau_f} = \frac{1}{\tau_{bulk}} + \frac{\nu_F}{\lambda} \]

\[ \lambda = \left[ \frac{2(1 - \Re)}{3\Re} \right] R_g \]

Real part of the dielectric function of Ni

![Graph showing the real part of the dielectric function of Ni for different thicknesses (50 Å, 105 Å, 210 Å, 800 Å).](image)

\[ (1) \]

![Graph showing the variation of \( \tau \) with thickness.](image)

\[ (2) \]
**Conclusions**

1. An Optical model was developed to determine the thickness of thin metal films.
2. Model was built to show that the thickness-dependent optical properties of thin metal films are correlated to the change in Drude free electron relaxation time.
3. The change in free electron relaxation time was traced to the change in grain boundary reflection coefficient and grain size.
Linear Optical Response of Materials

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- Phonon Absorptions
- Electronic Transitions
- Molecular Bond Vibrations
- Bandgap

Metals
Semiconductors
Dielectrics
Investigation of Optical Properties of BCB Wafer Bonding Layer used for 3D Interconnects via Infrared Spectroscopic Ellipsometry

2D Interconnects – 45 nm node

3D Interconnects – TSV


4ASM International
Why 3D Interconnects?

- Replacing long horizontal lines with short vertical interconnects
  - Addresses RC delay, crosstalk and power consumption
- Enables integration of heterogeneous devices & technologies (memory, logic, RF, analog, sensors)
  - Enables new functionalities
  - Cost reduction compared to SoC

Diagram:
- 3rd Level (thinned substrate)
- 2nd Level (thinned substrate)
- 1st Level after backgrinding
- Device layer / IMD
- BCB (Benzocyclobutene)
- Bonding Layer
- Substrate
Top wafer peeling due to air pockets in the BCB film

37% cross-linked BCB bond

Thinned TSV wafer

Handle wafer

Void

BCB

SEM cross-section image

SAM image

Dendritic structures
\[ (\Psi, \Delta) \rightarrow (n, t) \text{ when } k = 0 \Rightarrow \text{in a transparent region and determining thickness} \]

\[ t \Rightarrow (\Psi, \Delta) \rightarrow (n, k) \text{ in the entire spectrum} \]
The thermal curing of BCB polymers is a two step process:

1. Thermally activated opening of the BCB ring to form an o-quinodimethane intermediate.

2. The o-quinodimethane reacts with residual alkene groups in the via a Diels-Alder reaction, forming a tri-substituted tetrahydronaphthalene (THN).
IRSE Absorption Spectra of BCB

BCB \xrightarrow{1\text{st}} \text{o-quinodimethane} \quad + \quad \text{Residual alkene} \xrightarrow{2\text{nd}} \text{Trisubstituted THN}

- Si-O Stretch (1050 cm\(^{-1}\))
- Si-CH\(_3\) (1255 cm\(^{-1}\))
- Vinyl Rocking (1194 cm\(^{-1}\))
- Tetrahydronaphthalene (THN - 1498 cm\(^{-1}\))
- BCB Stretch (1472 cm\(^{-1}\))
- Vinyl moiety (985 cm\(^{-1}\))
% curing = \( 95 \left( \frac{A_{1498}}{A_{1255}} \right) \)

\( \frac{A_{1498}}{A_{1255}} \) Hardcured

Area = Peak × \( \frac{\text{F.W.H.M}}{\sqrt{2 \ln(2)}} \) × \( \sqrt{2\pi} \)
Ideal Bonded Wafer: 60% Cross-linked BCB Bond

<table>
<thead>
<tr>
<th>Hardbake</th>
<th>Cross Linking Level</th>
<th>Experiment Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temp °C</td>
<td>Time (min)</td>
<td>37%</td>
</tr>
<tr>
<td>190</td>
<td>10</td>
<td>42%</td>
</tr>
<tr>
<td>190</td>
<td>25</td>
<td>45%</td>
</tr>
<tr>
<td>190</td>
<td>40</td>
<td>45%</td>
</tr>
<tr>
<td>200</td>
<td>15</td>
<td>50%</td>
</tr>
<tr>
<td>200</td>
<td>25</td>
<td>50%</td>
</tr>
<tr>
<td>250</td>
<td>36 (sec)</td>
<td>60%</td>
</tr>
<tr>
<td>200</td>
<td>40</td>
<td>60%</td>
</tr>
<tr>
<td>250</td>
<td>64 (sec)</td>
<td>70%</td>
</tr>
<tr>
<td>250</td>
<td>2</td>
<td>70%</td>
</tr>
<tr>
<td>250</td>
<td>3.5</td>
<td>80%</td>
</tr>
</tbody>
</table>

Future Directions:

- Bonding using adhesive materials is relatively new in the semiconductor industry.
  - IRSE can aid in screening newly investigated materials.
  - IRSE will aid in process tuning and development.
Spectroscopic Ellipsometry of Porous Low-κ Dielectric Thin Films


Pores reduce the effective dielectric constant of the material

- Decrease signal propagation delays (faster switching speed)
- Reduction in crosstalk and power consumption
- Lower heat dissipation
- Pore volume fraction and pore size will effect the thermo-mechanical properties

**IBM (Porous SiCOH)**

- PECVD of dual-phase materials (matrix and organic precursors)
- UV cured to desorb porogens (organic precursor)

<table>
<thead>
<tr>
<th>Sample</th>
<th>( \kappa )</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SiCOH1</td>
<td>3.0</td>
<td>1000</td>
</tr>
<tr>
<td>SiCOH2</td>
<td>2.2-2.4</td>
<td>333</td>
</tr>
<tr>
<td>SiCOH3</td>
<td>2.2-2.4</td>
<td>363</td>
</tr>
</tbody>
</table>

**Novellus (ULK)**

- PECVD of porous low-\( \kappa \) with different dielectric constant

<table>
<thead>
<tr>
<th>Sample</th>
<th>( \kappa )</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ULK1</td>
<td>2.75</td>
<td>150</td>
</tr>
<tr>
<td>ULK2</td>
<td>2.65</td>
<td>150</td>
</tr>
<tr>
<td>ULK3</td>
<td>2.55</td>
<td>150</td>
</tr>
</tbody>
</table>
Bruggeman expression for effective medium approximation on porous SiCOH samples:

\[ f_a \frac{\varepsilon_a - \varepsilon}{\varepsilon_a + 2\varepsilon} + f_b \frac{\varepsilon_b - \varepsilon}{\varepsilon_b + 2\varepsilon} = 0 \]

<table>
<thead>
<tr>
<th>Pore Volume Fraction</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Control</td>
<td>0% 1055.0 0.2</td>
</tr>
<tr>
<td>333 nm</td>
<td>24.8 0.3 % 352.6 1.0</td>
</tr>
<tr>
<td>363 nm</td>
<td>23.8 0.1 % 379.5 0.4</td>
</tr>
</tbody>
</table>

Silicon

Silicon

**Graded BEMA Layer (590 nm)**

- **MSE**: 5.768
- **Thickness**: 386.982, 0.361 nm
- **Pore Volume**: 24.8, 0.3%

**Graded BEMA Layer (590 nm)**

- **MSE**: 6.559
- **Thickness**: 356.184, 0.773 nm
- **Pore Volume**: 24.862, 0.31%
Molecular Bond Vibrations (Novellus)

**Refractive Index (n) vs. Wavelength (nm)**

- \( \kappa = 2.75 \)
- \( \kappa = 2.65 \)
- \( \kappa = 2.55 \)

**Absorption Coefficient (1/cm) vs. Wavenumber (1/cm)**

- Si-O
- Si-CH\(_3\)

**Relative Carbon Concentration (%)**

\[
\text{Relative Carbon Concentration} = \frac{A_C}{A_O + A_C}
\]

**Area Calculation**

\[
\text{Area} = \text{Peak} \times \frac{\text{F.W.H.M}}{\sqrt{2\ln(2)}} \times \sqrt{2}
\]

<table>
<thead>
<tr>
<th>( \kappa )</th>
<th>( n )</th>
<th>Carbon (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.55</td>
<td>1.48</td>
<td>4</td>
</tr>
<tr>
<td>2.65</td>
<td>1.461</td>
<td>2.4</td>
</tr>
<tr>
<td>2.75</td>
<td>1.453</td>
<td>1.5</td>
</tr>
</tbody>
</table>

\( A_C \) - area under the Si-CH\(_3\) peak

\( A_O \) - area under the Si-O peak
Lorentz-Lorenz

\[ B_{ef} = \frac{3}{4\pi} \cdot \frac{(n_{ef}^2 - 1)}{(n_{ef}^2 + 2)} = \sum N_i \alpha_i \]

\[ P = \frac{B_{sat} - B_0}{B_{tol}} \]

Sample | Refractive Index \((n)\) | Porosity (%)
--- | --- | ---
\(\kappa = 2.55\) | 1.48 | 13.19
\(\kappa = 2.65\) | 1.461 | 11.76
\(\kappa = 2.75\) | 1.453 | 7.92

Toluene (low contact angle < 5°)

B\(_{ef}\) – effective polarizability
\(n_{ef}\) – effective refractive index (RI)
\(N_i\) - number of molecules
\(\alpha_i\) – molecular polarizability
\(n_{sat}\) – RI of film filled with toluene
\(n_{tol}\) – RI of toluene
\(n_o\) – RI of film without toluene
P - porosity
Dubinin and Radushkevitch (DR)

\[ V = V_0 \exp \left[ -\frac{1}{(\beta E_0)^2} \left( RT \ln \frac{P}{P_0} \right)^2 \right] \]

\[ \ln V = \ln V_0 - BA^2 \]

\[ A = RT \ln \left( \frac{P_0}{P} \right) \quad B = \frac{1}{(\beta E_0)^2} \]

\[ r = \frac{K}{2E_0} \]

A – adsorption potential  
R – universal gas constant  
V – adsorbate volume  
\( V_0 \) – total micro pore volume  
\( \beta \) – function of toluene only  
\( E_0 \) - solid characteristic energy towards a reference adsorbate  
K – empirical constant ≈ 12
SE can measure critical mechanical parameters (Young’s modulus, CTE)

- Young's modulus is a measure of the stiffness of the porous low-κ dielectric material
- A low CTE will prevent a connection failure between via/M1 and/or via/M2

Copper CTE ~ 20 x 10^{-6}/C
K. P. Mogilnikov and M. R. Baklanovz

\[ d = d_0 - k \ln \left( \frac{P}{P_0} \right) \]

\[ E = \frac{d_0 RT}{kV_L} \]

Sample | Porosity (%) | Pore radius (nm) | EP Young’s Modulus (GPa)
---|---|---|---
κ = 2.55 | 13.19 | 0.82 | 2.74
κ = 2.65 | 11.76 | 0.79 | 3.96
κ = 2.75 | 7.92 | 0.84 | 7.08

V_L – molecular volume
E – Young’s modulus
Free standing film (thermal expansion rate)

\[
\frac{1}{L_0} \frac{dL}{dT} = \alpha
\]

Film on substrate (CTE)

\[
\frac{1}{L_0} \frac{dL}{dT} = \left( \frac{1 + \nu_{\text{film}}}{1 - \nu_{\text{film}}} \right) \alpha_{\text{film}} - \left( \frac{2\nu_{\text{film}}}{1 - \nu_{\text{film}}} \right) \alpha_{\text{sub}}
\]

\( \nu_{\text{film}} = \text{Poisson's Ratio} = 0.25 \)

\( \alpha_{\text{substrate}} = 2.6 \times 10^{-6} \, / \, ^oC \)

Note: Fitting for the substrate expansion using the silicon temperature library (J.A.Woollam)
The following parameters were determined using SE.

- SICOH (IBM)
  - Porosity (BEMA)
  - Grading in porosity

- ULK (Novellus)
  - Carbon content
  - Porosity (EP)
  - Pore size
  - Young’s modulus
  - Coefficient of thermal expansion

Complementary techniques such as specular XRR, off-specular XRR and SAXS were also performed on these films. Both, the optical and x-ray metrology agreed reasonably well.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Thickness (nm)</th>
<th>$n$ (632.8 nm)</th>
<th>Carbon %</th>
<th>Porosity (%)</th>
<th>Pore radius (nm)</th>
<th>EP Young’s Modulus (GPa)</th>
<th>TER (10^{-6}/°C)</th>
<th>CTE (10^{-6}/°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\kappa = 2.55$</td>
<td>155.6</td>
<td>1.48</td>
<td>4</td>
<td>13.19</td>
<td>0.82</td>
<td>2.74</td>
<td>70.2</td>
<td>44.72</td>
</tr>
<tr>
<td>$\kappa = 2.65$</td>
<td>154.7</td>
<td>1.461</td>
<td>2.4</td>
<td>11.76</td>
<td>0.79</td>
<td>3.96</td>
<td>54.9</td>
<td>35.54</td>
</tr>
<tr>
<td>$\kappa = 2.75$</td>
<td>147.1</td>
<td>1.453</td>
<td>1.5</td>
<td>7.92</td>
<td>0.84</td>
<td>7.08</td>
<td>29.5</td>
<td>20.30</td>
</tr>
</tbody>
</table>
Linear Optical Response of Materials

(a) Intraband Absorptions
(b) Phonon Absorptions
(c) Molecular Bond Vibrations

Metals
Semiconductors
Dielectrics
Extension of Far UV spectroscopic ellipsometry studies of High-κ dielectric films to 130 nm

Absorption Cross-section

- Oxygen
- H2O
- N2

Wavelength (nm)

Oxygen / Water

Nitrogen
Linear Optical Response of Materials

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- **Molecular Bond Vibrations**
- **Bandgap**

**Materials**
- **Metals**
- **Semiconductors**
- **Dielectrics**
Metrology of Strain Engineered GaN/AlN/Si(111) Thin Films Grown by MOCVD

Substrate engineering consists of 4 major steps:
1) Growth of an epitaxial AlN buffer layer on Si
2) Implantation of AlN/Si with N⁺ ions to create a defective layer in Si below AlN buffer
3) Annealing of AlN/Si to recover any loss of crystallinity due to implantation
4) Growth of thick (2 µm) GaN on AlN/Si
IRSE of Substrate Engineered AlN Layers

(1) AlN/Si

(2) Implanted (60 keV N$^{14+}$)

(3) Annealed (1100 °C)

Bulk Si

AlN

Implanted

EMA Layer

Exp E 70° Si_AlN_Implanted_Annealed

Exp E 70° Si_AlN_Implanted

Exp E 70° Si_AlN

Implantation

E$_1$
- Resolution = 2 cm\(^{-1}\)
- \(E_1\) (TO) Bulk AlN = 666 cm\(^{-1}\)
- Isotropic model due to very thin AlN films (IR Probe)
- Tensile Biaxial Strain
- Broadening of the \(E_1\) (TO) phonon mode in implanted AlN is clear sign of presence of defects
- Not sensitive to the \(A_1\) (TO) due to c-plane orientation

<table>
<thead>
<tr>
<th>Sample List</th>
<th>(E_1) (TO) cm(^{-1})</th>
<th>(\gamma) (cm(^{-1}))</th>
<th>(\Delta \omega) (cm(^{-1}))</th>
<th>(d\omega_o/dP)</th>
<th>Stress (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si_AlN</td>
<td>662.2</td>
<td>0.08</td>
<td>19.5</td>
<td>3.8</td>
<td>0.84</td>
</tr>
<tr>
<td>Si_AlN_ Implanted</td>
<td>664.5</td>
<td>0.24</td>
<td>56.0</td>
<td>1.5</td>
<td>0.33</td>
</tr>
<tr>
<td>Si_AlN_Annealed</td>
<td>663.8</td>
<td>0.16</td>
<td>21.2</td>
<td>2.1</td>
<td>0.48</td>
</tr>
</tbody>
</table>
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Graphene
Semiconductors
Dielectrics
Spectroscopic Ellipsometry of CVD Graphene

Graphene
Surface Roughness
Glass

Van Hove Singularity

*Graphene’s infrared-to-visible absorbance: ~2.3%
Wafer Mapping - CVD Graphene on 300nm SiO₂/Si
Linear Optical Response of Materials

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- Metals
- Semiconductors
- Dielectrics
Temperature and thickness dependence of the dielectric function and interband critical points in ETSOI

Dielectric response of bulk Si and nanoscale silicon films in different

Advantages of SOI technology:
• Excellent isolation of active devices
• Lowers the parasitic capacitance
• Lower leakage current
• Faster device operation
• Lower power consumption
First Brillouin zone (truncated octahedron) of FCC Lattice

- [100] Direction: Γ Δ X
- [111] Direction: Γ Λ L
- [110] Direction: Γ Σ K

Critical Point
- Constant energy difference between the valence and conduction band.
- In optical physics terms – a high joint density of states.

Band structure of Si calculated from the \( \mathbf{k} \cdot \mathbf{p} \) method

\( \varepsilon_2 \): Imaginary part of the dielectric function

\( E_1 \): Electronic transitions

Direct space analysis:

Lorentzian line shape

\[ \epsilon = Ce^{i\beta}(E - E_g + i\Gamma)^{-\mu} \]

Double derivative of the Lorentzian line shape

\[ \frac{d^2 \epsilon}{dE^2} = \left\{ \begin{array}{ll} \mu(\mu + 1)Ce^{i\beta}(E - E_g + i\Gamma)^{-\mu - 2}, & \mu \neq 0 \\ Ce^{i\beta}(E - E_g + i\Gamma)^{-2}, & \mu = 0 \end{array} \right. \]

- \( C \) – amplitude
- \( \beta \) – phase factor
- \( E_g \) – threshold energy (ECP)
- \( \Gamma \) – lifetime broadening
- \( \mu \) – order of singularity

\( \mu = \frac{1}{2} \) (3D one-electron approximation)
\( \mu = 0 \) (2D one-electron approximation)
\( \mu = -\frac{1}{2} \) (1D one-electron approximation)
\( \mu = 1 \) (excitonic critical points)

Change in the dielectric function of c-Si nanoscale films at different thickness

Blue shift in the critical point energy is observed

A. Diebold et al., phys. stat. sol. (a) 205, 896 (2008)
Altering the optical response by changing the top dielectric layer: changes in quantum confinement and electron-phonon interaction
In-line optical metrology

Thickness dependent dielectric function

Silicon
SiO₂
SiO₂
Silicon

What does it mean to in-line metrology?
• A recipe which has thickness dependent optical properties
• A recipe which has top dielectric layer dependent optical properties

Surface dielectric dependent dielectric function

Silicon
SiO₂
SiO₂
SiO₂
Silicon

HfO₂
Silicon
SiO₂
Silicon
Outline

- Linear Optical Response of Materials
- Spectroscopic Ellipsometry
- Advanced Materials in the Semiconductor Industry
  - Photoreflectance
- Photoluminescence
- Conclusions
- Acknowledgements
Modulation spectroscopy (non-linear optical spectroscopy)

- Space charge layer at the surface due to Fermi level pinning
- Laser light produces carriers
- Carriers neutralize charge at the interface
- Modulation of light alters band bending
- Complex dielectric functions changes with band bending

Complementary technique to measure the shift in the energy and lifetime broadening of the $E_1$ critical point
Photoreflectance

\[
\frac{\Delta R}{R} (\hbar \omega) = \frac{R_{\text{off}} (\hbar \omega) - R_{\text{on}} (\hbar \omega)}{R_{\text{off}} (\hbar \omega)}
\]

Xenon source (probe)

CW Laser

532 nm (pump)

Chopped 1.38 k Hz

Monochromator

CCD

PR Spectrum

X,Y sample Stage

Filter
a & b are the Seraphin coefficients

Changes in the dielectric function due to the perturbation

Low field regime: Third Derivative Functional form:

$$\epsilon_2 \propto \Delta n_{CP}$$

A: Amplitude

Θ: Phase

$$E_{CP}:$$ Critical point

$$\Gamma:$$ Lineshape Broadening

n: Determined by type of CP

Photorelectance

 Photon Energy (eV)

E_1 \sim 3.39 \text{ eV}
Three transitions energies are (i) 3.19 eV, (ii) 3.30 eV and (iii) 3.45 eV.

Calculations show tensile strain of 1% in the strained Si overlayer.

This value is again in good agreement with the nominal tensile strain and with the values obtained from RS and Low Temp PhotoLuminescence.
Franz Keldysh Oscillations
Due to internal electric field in polar GaN

\[ \frac{\Delta R}{R} \propto \exp \left[ \frac{-2\Gamma \sqrt{E - E_g}}{(\hbar \Theta)^{3/2}} \right] \times \cos \left[ \frac{4}{3} \left( \frac{E - E_g}{\hbar \Theta} \right)^{3/2} + \phi \right] \frac{1}{E^2 (E - E_g)} \]

\[ F = \frac{(\hbar \Theta)^{3/2} \sqrt{2 \mu}}{e \hbar} \]

where \( \hbar \Theta \) is the electro-optic energy, \( \Gamma \) is the linewidth, \( \phi \) is the phase factor, \( F \) is the electric field, and \( \mu \) is the electron hole reduced mass (\( \mu = 0.2 \, m_e \)). The field estimated from the period of FKOs is 215 kV/cm (see Fig. 3). Such a huge
<table>
<thead>
<tr>
<th>Sample</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>%Sb</td>
<td>38.3</td>
<td>38</td>
<td>45.7</td>
<td>51</td>
<td>52.5</td>
</tr>
<tr>
<td>Thickness $d$ (nm)</td>
<td>41</td>
<td>72</td>
<td>50</td>
<td>72</td>
<td>41</td>
</tr>
<tr>
<td>$E_{\text{GHH}}$ (eV)</td>
<td>0.730</td>
<td>0.732</td>
<td>0.705</td>
<td>0.694</td>
<td>0.692</td>
</tr>
<tr>
<td>$E_{\text{GLH}}$ (eV)</td>
<td>0.681</td>
<td>0.681</td>
<td>0.689</td>
<td>0.695</td>
<td>0.696</td>
</tr>
<tr>
<td>$\Delta E_{\text{GHH-GLH}}$ (meV)</td>
<td>49</td>
<td>51</td>
<td>16</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>$F$ (kV/cm)</td>
<td>92</td>
<td>52</td>
<td>80</td>
<td>54</td>
<td>96</td>
</tr>
</tbody>
</table>

**Internal E Field**

**Chouaib, APL 93, (2008) 041913**

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Outline

- Linear Optical Response of Materials
- Spectroscopic Ellipsometry
- Advanced Materials in the Semiconductor Industry
- Photoreflectance
- Photoluminescence
- Conclusions
- Acknowledgements
Photoluminescence is used to study the changes in the indirect transitions due to quantum confinement and change in dielectric medium

Photoluminescence peak energy (2D)

\[ E = E_{\text{gap}} + E_{\text{QC}} - \frac{R_y}{n - \frac{1}{2}}^2 + \frac{\hbar^2 (k_x^2 + k_y^2)}{2M} \]

\[ E_{\text{QC}} = \frac{\hbar^2 \pi^2}{2ML^2} \]

\[ R_y = \frac{m^*}{2} \left( \frac{e^2}{4\pi\varepsilon_0 \hbar} \right)^2 \rightarrow \text{Rydberg} \]

Band structure of Si calculated from the \( \mathbf{k} \cdot \mathbf{p} \) method\(^1\)

As the power is increased, at high densities, and at low temperatures the free excitons condense to form a liquid phase.

This liquid phase manifests itself in the formation of EHD (Electron-hole droplets) – a broad feature in luminescence.

BE – Binding Energy
Fig. 2. PL mapping on (a) SIMOX, (b) Unibond®, and (c) ELTRAN® wafers with $t_{\text{SOI}} = 170\,\text{ - }200\,\text{nm at room temperature}$: Upper and lower figures are on top Si layers and substrates, respectively.
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Conclusions

- A wide range of wavelengths makes Spectroscopic Ellipsometry a very powerful method capable of measuring more than just thickness and refractive index.

- Non Linear Optical methods such as Photoreflectance and Photoluminescence provide information not available from spectroscopic ellipsometry.