OPTICAL PROPERTIES OF SILICON NITRIDE THIN FILMS DEPOSITED BY REACTIVE DC MAGNETRON SPUTTERING

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Outline:

• Purpose of the Study
• Properties and Applications of SiN Thin Films
• Coating Methods
• Experimental
• Characterization
• Results and Discussion
Purpose:

- Changing the composition of the coatings by modifying the reactive gas flow ratio,
- Investigating the effects of the composition change on structural and optical properties.
- SiN films are mainly studied on their optical transmittance.
- This study is unique in terms of target material, reactive gas types, flow rates and application of Tauc rule.
Silicon nitride is a semiconductor and has:

- High strength,
- High thermal stability,
- High chemical inertness,
- Good corrosion resistance,
- Good mechanical and dielectric properties,
- High transparency,
- Behaves as a passivation layer for microchip technologies against water molecules and sodium ions.

All these properties make silicon nitride very useful for industrial applications, microelectronics and optoelectronics.
Coating Methods:

SiN films can be deposited by a variety of techniques,

- Laser ablation,
- Chemical vapor deposition,
- Ion implantation,
- Ion beam sputtering,
- Reactive magnetron sputtering.

- From the various possible choices, magnetron sputtering appears to be very attractive, due to its relative simplicity, low depositing temperature, high attainable deposition rates and wide acceptance by industry.
Experimental:

• Substrates

• Vacuum and etching

• Coating
Substrates:

• **Corning glasses** for optical studies
  (LT1001740, 26 mm x 76 mm x 1 mm)

• **M2 high speed steels** for other studies
  (% 0,9 C, % 4,1 Cr, %5 Mo, % 1,9 V, % 6,4 W)
Top Down Schematic View of TSD 350 PCVD Coating Chamber:

1. Vacuum Chamber
2. CMP-150 Magnetron cathode
3. Plasma Generator
4. Substrate Holder
5. Target Material
Vacuum and Etching:

- Base pressure of $1 \times 10^{-5}$ Pa (Rotary and turbomolecular pump combination)
- %99,999 purity argon gas for generating plasma
- 0.2 Pa working pressure
- Plasma booster for etching
- Bias etching 50 V - 250 V
Coating:

• Target Material: 150 mm radius, 7 mm thickness 99.999% purity single crystal Si
• Reactive gas: N₂
• Ar & N₂ total gas flow of 20 cm³/min
• N₂ gas flow rate 1-10 cm³/min
### Deposition Parameters:

<table>
<thead>
<tr>
<th></th>
<th>SiN 1</th>
<th>SiN 2</th>
<th>SiN 3</th>
<th>SiN 4</th>
<th>SiN 5</th>
<th>SiN 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ar Gas Flow [cm³/min]</td>
<td>19</td>
<td>18</td>
<td>16</td>
<td>15</td>
<td>13</td>
<td>10</td>
</tr>
<tr>
<td>N₂ Gas Flow [cm³/min]</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>5</td>
<td>7</td>
<td>10</td>
</tr>
<tr>
<td>Deposition Time [min]</td>
<td>40</td>
<td>40</td>
<td>40</td>
<td>50</td>
<td>70</td>
<td>100</td>
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</table>

**Base Pressure**: 1x10⁻⁵ Pa

**Working Pressure**: 0.2 Pa

**Deposition Temp.**: 40±5°C

**Sputtering Power**: 500 W

**Cathode Voltage**: 710±80 V

**Cathode Current**: 0.75±0.09 A

**Bias Voltage**: 50 V
Characterization:

- **Thickness & Microstructure**: SEM / JEOL JSM 7000F SEM
- **Chemical composition**: EDS
- **Optical Properties**: Spectrophotometer / NKD 7000 (Aquila, UK) Pro-Optix software
- **Band Gap Calculations**: Tauc Rule
Profile and Thickness

All the thicknesses are in the standard deviation range of 1000±200nm.

Representative

(M2 Steel)
EDS Analysis by Atomic Percent

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Gas Flow Rate (cm³/min)</th>
<th>at%</th>
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</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>N</td>
</tr>
<tr>
<td>SiN 1</td>
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<tr>
<td>SiN 2</td>
<td>2</td>
<td>25.02</td>
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<tr>
<td>SiN 3</td>
<td>4</td>
<td>26.89</td>
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<tr>
<td>SiN 4</td>
<td>5</td>
<td>47.56</td>
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<tr>
<td>SiN 5</td>
<td>7</td>
<td>55.65</td>
</tr>
<tr>
<td>SiN 6</td>
<td>10</td>
<td>58.59</td>
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</table>
Optical Transmittance

![Graph showing optical transmittance vs wavelength for different samples.](image-url)
Optical Reflectance

![Graph showing optical reflectance data for different nitride compositions.](image)
Band Gap

- **Conduction Band**
- **Valence Band**

**INSULATOR**

**SEMICONDUCTOR**

**CONDUCTOR**
Calculation of Band Gap

\[ E = \frac{hc}{\lambda} \]

\[ \tilde{n} = n - ik \]
- \( n \) = Real index of refraction
- \( k \) = Extinction coefficient

\[ \sqrt{\alpha(h\nu)h\nu} = C_{\text{Tauc}}(h\nu - E_{\text{g Tauc}}) \]

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

\((\alpha h\nu)^{1/2} - (h\nu)\) graph
Calculation of Band Gap
# Indirect Band Gaps

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Nitrogen Gas Flow (cm³/min)</th>
<th>Band Gap (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SiN 1</td>
<td>1</td>
<td>1.62</td>
</tr>
<tr>
<td>SiN 2</td>
<td>2</td>
<td>1.63</td>
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<tr>
<td>SiN 3</td>
<td>4</td>
<td>1.91</td>
</tr>
<tr>
<td>SiN 4</td>
<td>5</td>
<td>1.54</td>
</tr>
<tr>
<td>SiN 5</td>
<td>7</td>
<td>2.99</td>
</tr>
<tr>
<td>SiN 6</td>
<td>10</td>
<td>3.07</td>
</tr>
</tbody>
</table>
Band Gap vs. Gas Flow

![Graph showing the relationship between Band Gap (eV) and % N₂](image)
Results:

• Homogeneous, dense and well-adherent silicon nitride thin films with thicknesses around 1000 nm with variable compositions were successfully deposited on glass and steel substrates by reactive DC magnetron sputtering.

• A spectrophotometer with inline software capability was used for determining the transmittance, reflectance and extinction coefficient values of silicon carbide films. Tauc rule was used for determining the optical band gap values.

• Increase in nitrogen concentration resulted a dramatic increase in transmittance and decrease in reflectance values.

• The increase in N concentration results in an increase in optical band gap values. The optical gaps range from 1.54 to 3.07 eV.
Conclusions

- **Nitrogen** concentration in SiN thin films has significant influence on both **optical constants** and **optical band gaps**.

- Band gap increase improves the **insulating ability** of these semiconductor films.

- **Transmittance** and **reflectance** values of SiN films could **easily be tailored** by modifying **Si** and **N concentrations** in the coating, for the similar film thicknesses.

- These SiN thin films can be used either as a **transmitter** system or **reflector** system for designated purposes (Optoelectronic and electronic applications in such devices as solar cells, phototransistors, image sensors, light emitting devices etc.).
Thank You For Your Attention

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