Beyond $\text{SiO}_x$ for Hole-Selective Poly-Si Passivating Contacts
- The potential of $\text{SiN}_x$ or $\text{AlO}_x$

Shona McNab, Peter Wilshaw, Ruy Sebastian Bonilla
Outline

• Poly-Si contacts – or ‘TOPCon’
• Current limitations with SiO$_x$
• Benefits of SiN$_x$ and AlO$_x$

• Fabrication
• Transport Properties
• Passivation Properties
• Comparison with other work
• Summary
TOPCon Silicon Cells

**Tunnel Oxide Passivated Contact**

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**Trend: share of cell technologies**

<table>
<thead>
<tr>
<th>Year</th>
<th>Share (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2023</td>
<td>50%</td>
</tr>
<tr>
<td>2024</td>
<td>45%</td>
</tr>
<tr>
<td>2025</td>
<td>40%</td>
</tr>
<tr>
<td>2026</td>
<td>35%</td>
</tr>
<tr>
<td>2027</td>
<td>30%</td>
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<tr>
<td>2028</td>
<td>25%</td>
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<td>2029</td>
<td>20%</td>
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<td>2030</td>
<td>15%</td>
</tr>
<tr>
<td>2031</td>
<td>10%</td>
</tr>
<tr>
<td>2032</td>
<td>5%</td>
</tr>
<tr>
<td>2033</td>
<td>0%</td>
</tr>
</tbody>
</table>

- **Topcon**: 50% in 2023, decreasing to 0% in 2033
- **PERC**: 45% in 2023, decreasing to 5% in 2033
- Other Technologies: increasing share from 0% in 2023 to 100% in 2033

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What comes next for TOPCon?

- SiO$_x$ poly-Si hole contacts
  - Both Sides passivated contacts
    → Potential for higher efficiency
  - So far less effective than electron contacts
    → Why?

Note: parasitic absorption from poly-Si on the front – not considered today!
Limitations of SiO\textsubscript{x}: Part 1
- Hole Transport Properties

• Tunnelling Current

 Thickness Barrier height

\[ \rho_c < 100 \text{ m}\Omega \cdot \text{cm}^2 \]

- Contact Resistivity [m\(\Omega\)cm\(^2\)]

- p-type SiO\textsubscript{x} hole contacts rely on pinhole conduction

\[ \text{SiO}_2 (p\text{-type}) \quad \text{SiO}_2 (n\text{-type}) \]

1 R. Basnet Appl. Phys. Rev. (2024), 11, 011311
S. McNab AIP Conference Proceedings, (2022), 020013
Limitations of SiO$_x$: Part 2
- P-type Passivation Properties

- Boron is more soluble in SiO$_x$ than Phosphorus:
  - Deeper diffusion – more Auger recombination
  - Boron in SiOx introduces defects – higher $D_{it}$

$\rightarrow$ More recombination

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1 Dan MacDonald, SPREE Seminar (2023)- https://www.youtube.com/watch?v=0dYnuhXTGXw
The Benefits of SiN$_x$ and AlO$_x$: Part 1
- Lower VBO

XPS VBO measurements

Tunnelling current Calculations

\[ \rho_c < 100 \text{ m}\Omega \cdot \text{cm}^2 \]

\[ \text{Thickness [nm]} \]

\[ \text{Contact Resistivity [m}\Omega\text{cm}^2] \]

2 S. McNab AIP Conference Proceedings, (2022), 020013

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The Benefits of SiN$_x$ and AlO$_x$: Part 2
- Boron diffusion profile

ECV Doping Profile

- SiN$_x$ blocks diffusion
- SiO$_x$ and AlO$_x$ deep boron diffusion

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SiOx has very little charge
AlOx has a negative charge
SiNx has a positive charge

Why is this important?

The Benefits of SiN$_x$ and AlO$_x$: Part 3

Field effect passivation?
AlO$_x$ has a negative charge – can it help?

Sentaurus TCAD Simulations

SiN$_x$ or AlO$_x$ Poly-Si Contacts

**Promise:**
- **Lower VBO** enables more tunnelling conduction
- SiN$_x$ **boron blocking** should reduce Auger recombination
- AlO$_x$ **negative charge** can add Field effect passivation

**Questions:**
- Can we fabricate these layers at the thickness and uniformity required
- Does the promise translate to real devices
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Fabrication Process

~2 nm Dielectric

$\text{p-Si}$

ALD $\text{AlO}_x$

PECVD $\text{SiN}_x$

Ex-situ Ellipsometry

Doped a-Si deposition
High T Anneal
$\text{SiN}_x$ Hydrogenation

*Limited samples so focus on understanding

1 S. McNab, Submitted
Dielectric layers for Poly-Si deposition

- Why RCA2 SiO$_x$?
  - Reasonable chemical passivation
  - Very thin → limited effect on the tunnelling conduction
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Contact resistivity: $\rho_c = (R_{tot} - R_{spread})A_c$

$R_{tot} = \left[\frac{dI}{dV}\right]_{V \equiv 0}$

- $\rho_c < 100 \text{ m}\Omega \cdot \text{cm}^2$
- Is it actually tunnelling?
Understanding Transport Mechanisms

• Temperature Dependent IV measurements

\[ \rho_{\text{tun}} = \frac{n k_B}{q A^* T} \cdot \exp\left(\frac{q \varphi_B}{kT}\right) \cdot P_t \]

\[ \rho_{\text{pin}} = \frac{1}{N_{\text{pin}}} \cdot \frac{\rho_B(T)}{2\pi r_{\text{pin}}} \cdot \arctan\left(\frac{2t_{\text{waf}}}{r_{\text{pin}}}\right) \]

850 °C Anneal

\[ N_{\text{pin}} \approx 10^8 \text{ cm}^{-2} \]

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Understanding Transport Mechanisms

- Batch 1a: Adjust anneal Temperature

- 800 °C anneal shows a purely tunnelling fit
- >850 °C has a high pinhole density
- Pinholes are not required for $\rho_c < 100 \text{ m}\Omega \cdot \text{cm}^2$
- But they might form anyway!
Outline

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• **Passivation Properties**
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Passivation

- Low $iV_{OC}$ compared to SiO$_x$ control
- AlO$_x$ too low to even measure!

- Why?

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interface.materials.ox.ac.uk shona.mcnab@materials.ox.ac.uk 21
Characterising Passivation: Uniformity

Severe inhomogeneity issues – but some areas with high passivation

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Characterising Passivation: $Q_f$ and $D_{it}$

- Thick dielectrics
- How do the properties of <2nm dielectrics compare
- Difficult to measure due to high conductivity

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Characterising Passivation: \( Q_f \) and \( D_{it} \)

- Surface Photovoltage
- No direct contact to the dielectric
  - Prevents conduction

- Effect of \( D_{it} \) and \( Q_f \) difficult to deconvolute

\[ +ve \ Q_f +ve \ Q_f -ve \ Q_f \]

1 S. McNab *IEEE Journal of Photovoltaics*, (2022), 1-11
Characterising Passivation: $Q_f$ and $D_{it}$

- CV is commonly used for thick dielectrics
  - $Q_f$ shifts curve left/right
  - $D_{it}$ changes the slope
- Sensitive to interface charge
- High conductivity prevents an accurate CV measurement

Capacitance-Voltage Measurements

![Graph showing capacitance-voltage measurements with labels for $Q_f$ and $D_{it}$, and a note on 'S-shape' behavior for 2 nm SiN and an expected fit.](image-url)
Characterising Passivation: $Q_f$ and $D_{it}$

Adapted CV analysis

- High Quality CV obtained
- $Q_f \times 10^{12}$ [q/cm$^2$]
- $D_{it} \times 10^{12}$ [cm$^2$]

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<thead>
<tr>
<th>Dielectric</th>
<th>$Q_f \times 10^{12}$</th>
<th>$D_{it} \times 10^{12}$</th>
</tr>
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<tbody>
<tr>
<td>RCA2 SiO$_x$</td>
<td>0.7</td>
<td>0.5</td>
</tr>
<tr>
<td>3s SiN</td>
<td>0.65</td>
<td>0.6</td>
</tr>
<tr>
<td>RCA2 + 3s SiN</td>
<td>1</td>
<td>0.4</td>
</tr>
<tr>
<td>10 cycles AlOx</td>
<td>-0.4</td>
<td>0.4</td>
</tr>
<tr>
<td>RCA2 + 10 AlOx</td>
<td>-3.2</td>
<td>2</td>
</tr>
</tbody>
</table>

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Characterising Passivation: $Q_f$ and $D_{it}$

Adapted CV analysis

- $\sim 2$ nm Dielectric

### Dielectric

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<tr>
<td>10 cycles AlO$_x$</td>
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<td>0.4</td>
</tr>
<tr>
<td>RCA2 + 10 AlO$_x$</td>
<td>-3.2</td>
<td>2</td>
</tr>
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Poly-Si Doping

- $10^{19}$ cm$^3$
- $10^{20}$ cm$^3$
- $10^{21}$ cm$^3$
Improved Passivation

Takeaways from Batch 1
• Tunnelling contacts are possible ✓
• Siₙ blocks boron ✓
• RCA2+AlOₓ has high -ve charge ✓
• High pinhole density ❌
• Uniformity issues ❌
• Used anneal optimised for SiOₓ

For Batch 2
• Varied anneal conditions
• Improved RCA2 processing and wafer handling
• Focus on most promising interlayers

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Batch 2 after hydrogenation
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Comparison to other work

![Graph showing comparison to other work](image-url)
Summary

• Potential benefits of PECVD SiN$_x$ and ALD AlO$_x$ as hole selective poly-Si tunnelling contacts

• Developed Methods for Characterising $Q_f$ and $D_{it}$ of 2nm dielectrics

• Significant improvement in 2 batches:
  • SiN$_x$ $iV_{OC}$ 668 → 699 mV
  • AlO$_x$ shows promise before poly-Si
Acknowledgements

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XPS data

• SiNx stoichiometry – low N concentration, close to SiOx

• AIOx – significant increase in Al concentration