New Non-Pyrophoric Al Precursor for the ALD of Al₂O₃: Influence of Purity Grade on Silicon Surface Passivation

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1. Introduction

Al₂O₃ deposited by atomic layer deposition (ALD) is known to provide excellent surface passivation of crystalline silicon (c-Si) solar cells [1,2]. However, metal impurities in passivation layers can significantly affect the cell’s efficiency [3]. A potential source of these impurities is the precursor gas used to deposit the layers. Therefore, we have investigated the effect of precursor purity on the surface passivation of Al₂O₃. The most commonly-used Al precursor is trimethylaluminium (TMA), which is a pyrophoric liquid. We recently reported the use of dimethylaluminium isopropoxide (DMAI) as a safer, non-pyrophoric alternative [4], where it was shown to give comparable results to TMA with respect to effective lifetimes in c-Si. We present here the use of DMAI spiked with Fe to test the significance of precursor purity.

2. Aluminium Precursor

<table>
<thead>
<tr>
<th>Physical State (R.T.P.)</th>
<th>Liquid</th>
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</thead>
<tbody>
<tr>
<td>Melting Point</td>
<td>&lt; R.T.</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>186 °C</td>
</tr>
<tr>
<td>Vapour Pressure</td>
<td>9 Torr at 66.5 °C</td>
</tr>
<tr>
<td>Decomposition Temp.</td>
<td>~370 °C</td>
</tr>
<tr>
<td>Pyrophoric</td>
<td>No</td>
</tr>
</tbody>
</table>

Dimethylaluminium isopropoxide (DMAI)

Purity Levels
- Unspiked (99.999%)
- 5 ppm Fe
- 500 ppm Fe

3. Experimental Details

<table>
<thead>
<tr>
<th>Substrates</th>
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<td>Double-side-polished floatzone Si</td>
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</tbody>
</table>

Effective Lifetime Measurements
- Sinton WCT-100 Photoconductance tool

4. Effective Lifetime (τₑff) Measurements

- Plasma-Enhanced ALD
  - p-type c-Si
  - n-type c-Si

- Thermal ALD
  - p-type c-Si
  - n-type c-Si

5. Recombination Velocities (Sₑff,max)

Fig. 1. Variation of effective lifetimes with Fe content for plasma-enhanced ALD films.

Fig. 2. Variation of effective lifetimes with Fe content for thermal ALD films.

6. ToF-SIMS Measurements

- Fe mainly observed in the Al₂O₃ layer, nearer the surface.
- Fe in the layer increases during firing.
- There is possibly some diffusion of Fe to the interface.

7. Conclusions

- Samples prepared using plasma-enhanced ALD were more affected by the presence of Fe than thermal ALD.
- The plasma-enhanced ALD samples were more affected by firing than the thermal ALD samples.
- The highest lifetimes were obtained by annealing (not firing) the plasma-enhanced ALD samples.
- n-type c-Si was more affected by the Fe than p-type.
- For n-type substrates, the presence of Fe reduces the effective lifetimes after firing.
- Up to 5 ppm Fe in the Al precursor can be considered non-detrimental to the effective lifetimes on p-type c-Si.


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