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New, Non-Pyrophoric Al-Precursor for the ALD of Al_2O_3: Influence of Purity Grade on Silicon Surface Passivation

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Al_2O_3 by atomic layer deposition (ALD) is known to provide excellent surface passivation of crystalline silicon (c-Si) solar cells.[1,2] Metal impurities in passivation layers can significantly affect the cell's efficiency.[3] A potential source of these impurities are the precursor gases used to deposit the layers. Therefore, we have investigated the effect of precursor purity on the surface passivation of Al_2O_3. The most commonly-used Al precursor is trimethylaluminium (TMA), which is a pyrophoric liquid. We recently reported the use of dimethylaluminium isopropoxide (DMAi, Table 1) as a safer, non-pyrophoric alternative to TMA.[4] We present here the use of DMAi spiked with iron to test the significance of precursor purity.

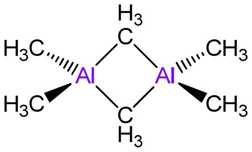
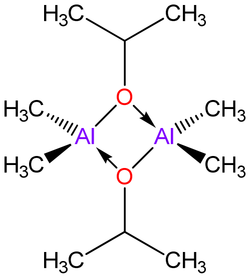
30 nm Al_2O_3 was deposited onto *n*- and *p*-type double-side-polished 4" c-Si floatzone wafers (~3.5 and ~2.2 Ω.cm, respectively) using plasma-enhanced ALD at 200 °C.[4] DMAi (purity = 99.999%) was used as the pure precursor and this was compared with batches spiked with 5 ppm and 500 ppm Fe. Effective carrier lifetimes were measured for as-deposited films, after annealing (10 min, 400 °C under N_2) and after high temperature annealing designed to mimic the contact "firing" process (5 s, 800 °C under N_2). Annealing afforded lifetimes in the order of 1 ms in all cases, but firing reduced this to ~10 and ~100 µs for *n*- and *p*-type Si, respectively. For the annealed samples, the maximum surface recombination velocities ($S_{eff,max}$, injection level = 5×10^{14} cm^{-3}) were 2.9 and 6.2 cm/s for *n*- and *p*-type Si, respectively (Fig. 1), which are comparable to those obtained when TMA was the Al precursor.[2] These values were higher when Fe-spiked DMAi was used to deposit the 30 nm thick layer. For DMAi containing 5 ppm Fe, $S_{eff,max}$ values of 16.9 and 7.3 cm/s (*n*- and *p*-type, respectively) were obtained after annealing, which still demonstrates a good level of passivation for c-Si solar cells. However, for the 500 ppm Fe-spiked DMAi, $S_{eff,max}$ values of 41.54 and 20.8 cm/s clearly showed a detrimental effect, suggesting a negative influence of a high concentration of Fe.

Using these results, we show here the potential of DMAi as a viable precursor for passivation and discuss the importance of precursor purity for use on c-Si.

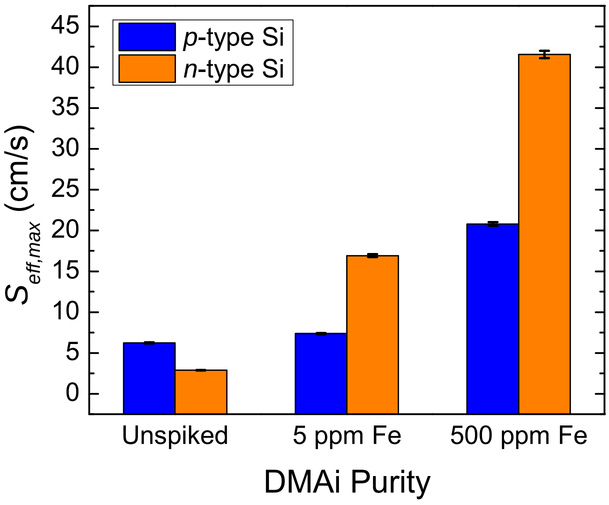
1. B. Hoex *et al.*, *Appl. Phys. Lett.*, **89**, 042112 (2006).
2. G. Dingemans *et al.*, *Phys. Status Solidi RRL*, **4**, 10 (2010).
3. C. A. Wolden *et al.*, *J. Vac. Sci. Technol. A*, **29**, 030801 (2011).
4. S. E. Potts *et al.*, *J. Vac. Sci. Technol. A*, **30**, in press (2012). DOI: 10.1116/1.3683057.

Explanatory Page

Table 1. A comparison of the general properties of the TMA and DMAi precursors.

Precursor Property	TMA	DMAi
Structural Formula	 Dimeric up to ~70 °C	
Physical State (R.T.P.)	Liquid	Liquid
Melting Point	15 °C	<R.T.
Boiling Point	125 °C	172 °C
Vapour Pressure	9 Torr at 16.8 °C	9 Torr at 66.5 °C
Decomposition Temperature	~330 °C[5]	~370 °C[6]
Pyrophoric	Yes	No

5. D. W. Squire *et al.*, *J. Vac. Sci. Technol. B*, **3**, 1513 (1985).
6. S. Y. Lee *et al.*, *Appl. Surf. Sci.*, **222**, 234 (2004).



$$S_{eff,\max} = \frac{d_W}{2\tau_{eff}}$$

d_W = wafer thickness
τ_{eff} = effective lifetime, taken at an injection level of 5×10^{14} cm^{-3}.

Figure 1. Maximum surface recombination velocities ($S_{eff,max}$) at an injection level of 5×10^{14} cm^{-3} for *p*- and *n*-type floatzone wafers (~2.2 and ~3.5 Ω.cm, respectively), coated with 30 nm Al_2O_3 by plasma-enhanced ALD using DMAi at 200 °C then annealed at 400 °C for 10 min under N_2.