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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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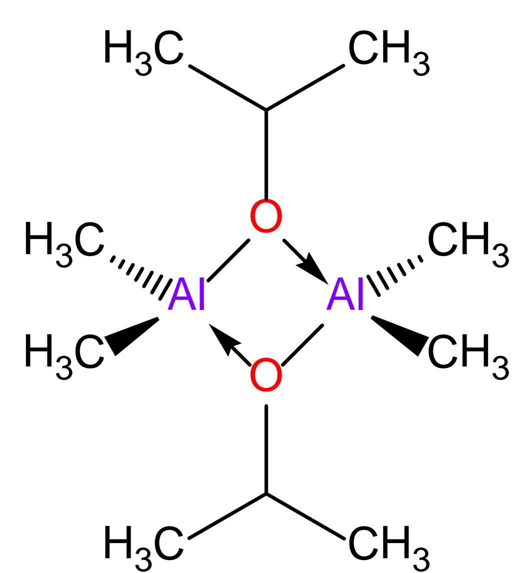
1. Introduction

Al_2O_3 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 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) 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



Dimethylaluminium isopropoxide (DMAI)

Physical State (R.T.P.)	Liquid
Melting Point	< R.T.
Boiling Point	186 °C
Vapour Pressure	9 Torr at 66.5 °C
Decomposition Temp.	~370 °C
Pyrophoric	**No**

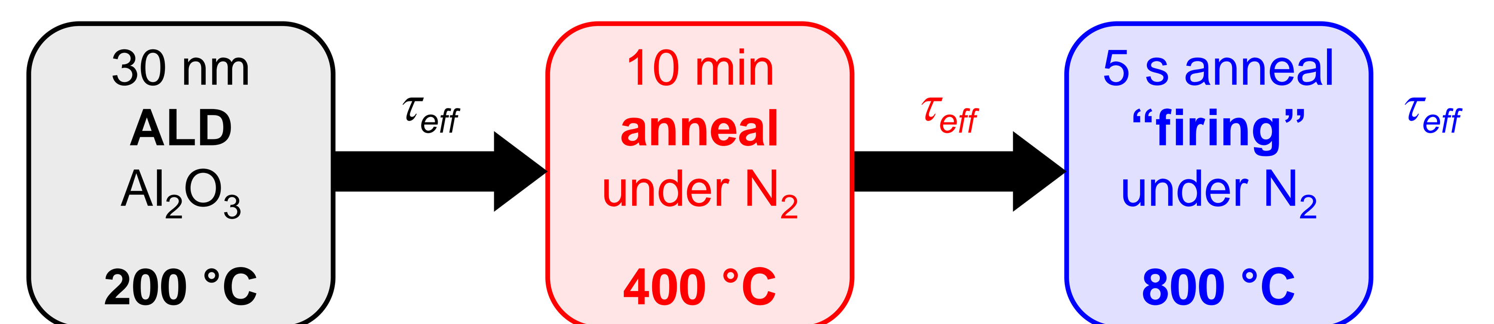
Purity Levels
- Unspiked (99.999%)
- 5 ppm Fe
- 500 ppm Fe

3. Experimental Details

ALD
- Oxford Instruments OpAL™ reactor
- Plasma and thermal ALD

Effective Lifetime Measurements
- Sinton WCT-100 Photoconductance tool

Substrates
- Double-side-polished floatzone Si
- *n*-type (~3.5 Ω.cm)
- *p*-type (~2.0 Ω.cm)
- HF-dip before depositions



4. Effective Lifetime (τ_{eff}) Measurements

Plasma-Enhanced ALD

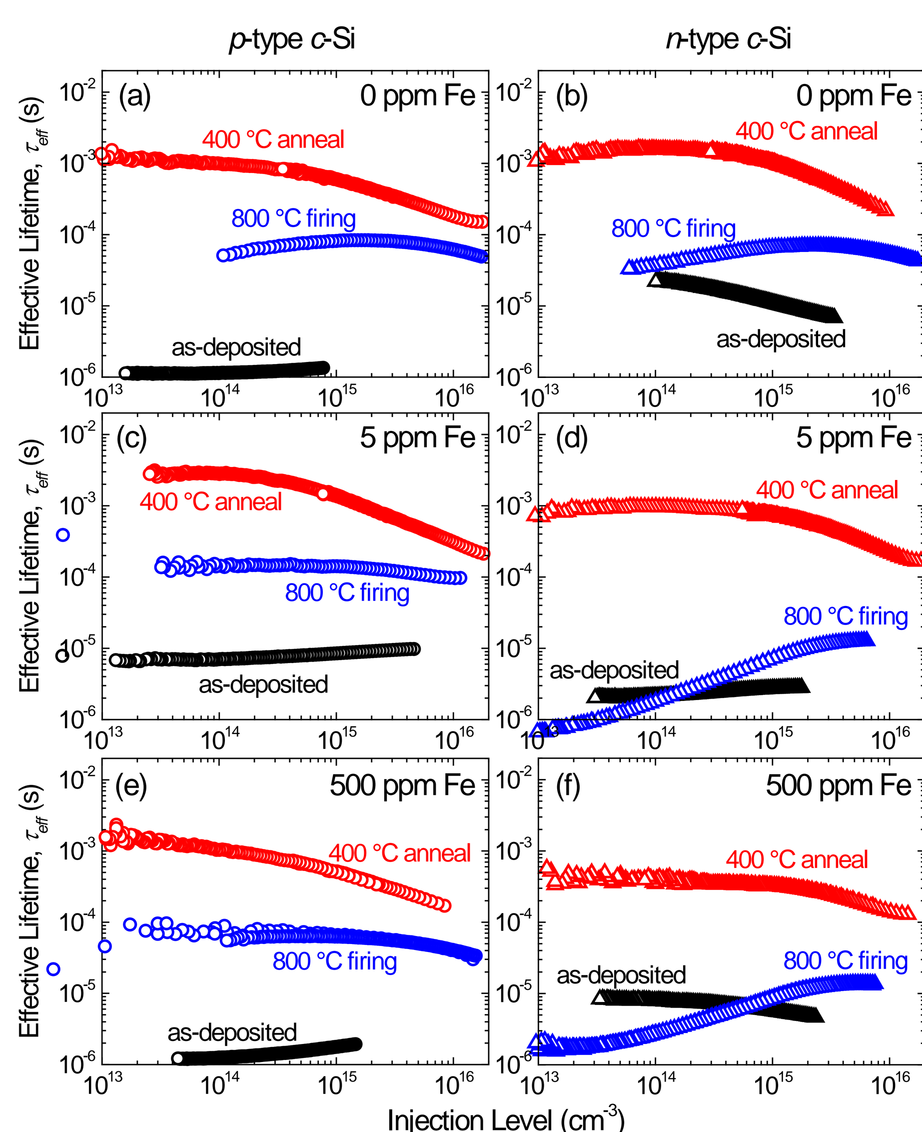


Fig. 1. Variation of effective lifetimes with Fe content for plasma-enhanced ALD films.

Thermal ALD

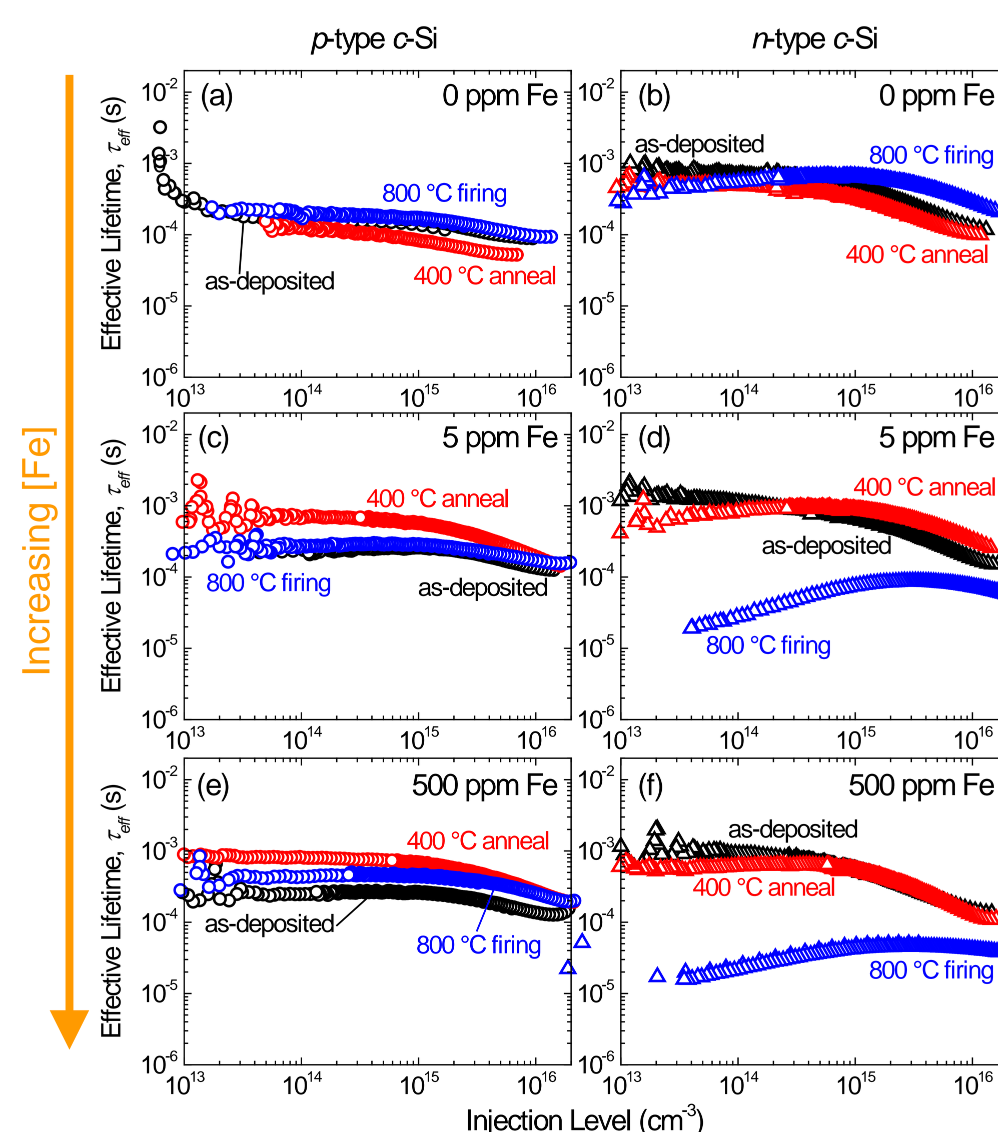


Fig. 2. Variation of effective lifetimes with Fe content for thermal ALD films.

5. Recombination Velocities ($S_{eff,max}$)

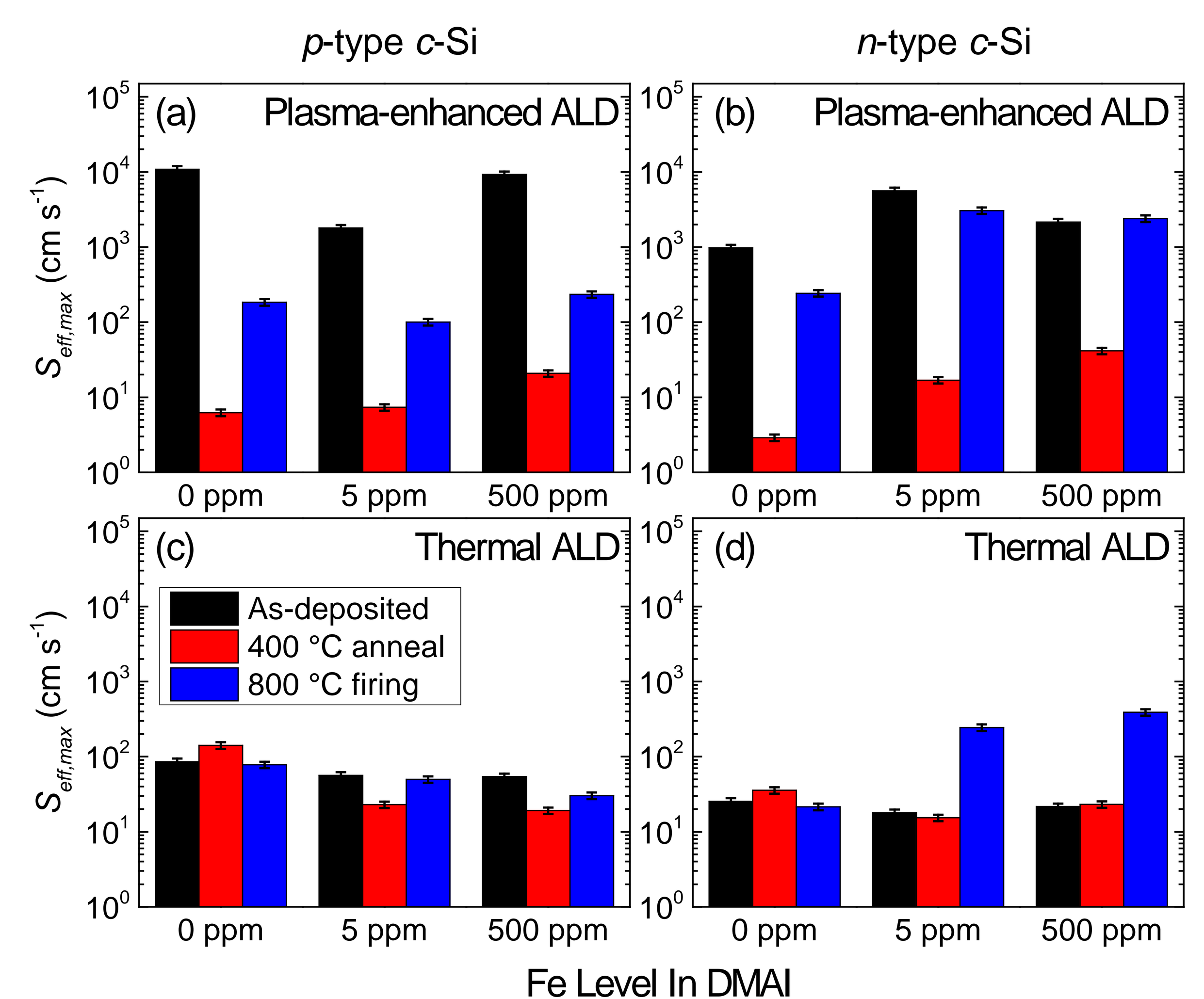
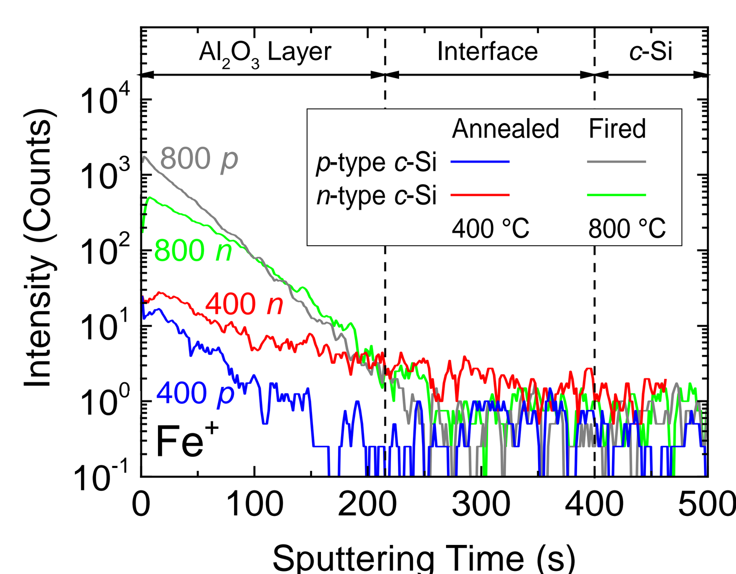


Fig. 3. Surface recombination velocities for n- and p-type c-Si showing the effect of Fe content in the DMAI precursor.

6. ToF-SIMS Measurements

- Fe mainly observed in the Al_2O_3 layer, nearer the surface.
- Fe in the layer increases during firing.
- There is possibly some diffusion of Fe to the interface.

Fig. 4 (right). ToF-SIMS Fe^+ ion profile for annealed and fired Al_2O_3 films on n- and p-type c-Si.



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.**

[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**, 021505 (2012).

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