Excellent silicon surface passivation by TiO_x: aiming for electron selectivity by atomic layer deposition

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Passivating contact criteria[1-3]

1. Contact resistivity
2. Passivation
3. Transparency
4. Full-area lean processing

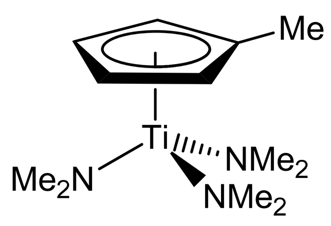
Possible electron-selective material: TiO_x

1. Small ΔE_c & large ΔE_v[4]
2. Atomic layer deposition (ALD) precursors: $TiCl_4$[5,7-9] and TTIP[6,10] → optimal choices?
3. Wide bandgap
4. High η (20-22%) solar cells[5-9]

Research questions: optimal ALD TiO_x recipe, precursor, and annealing treatment?

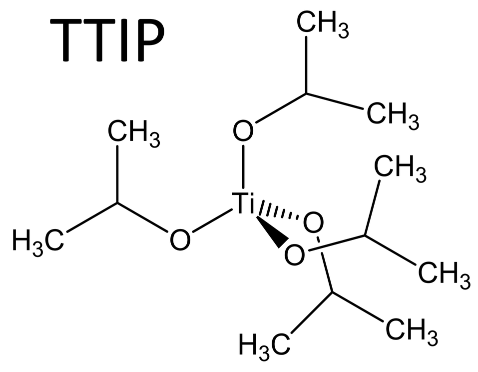
Experimental variables

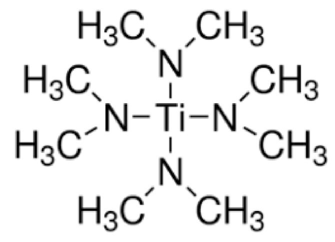
1. Precursors & oxidants
2. Temperature (growth & annealing)
3. Film thickness



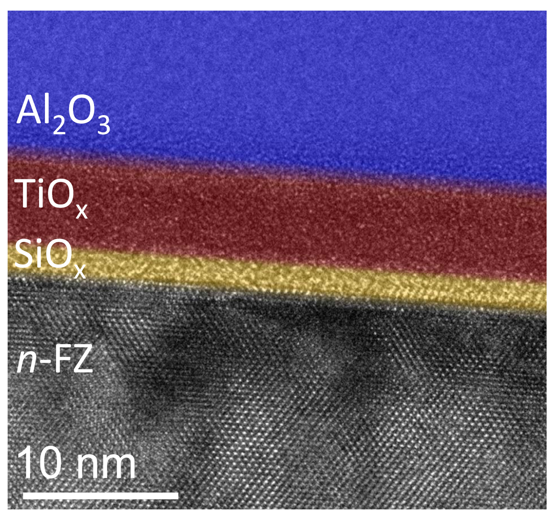
$Ti(Cp^{Me})(NMe_2)_3$

TTIP



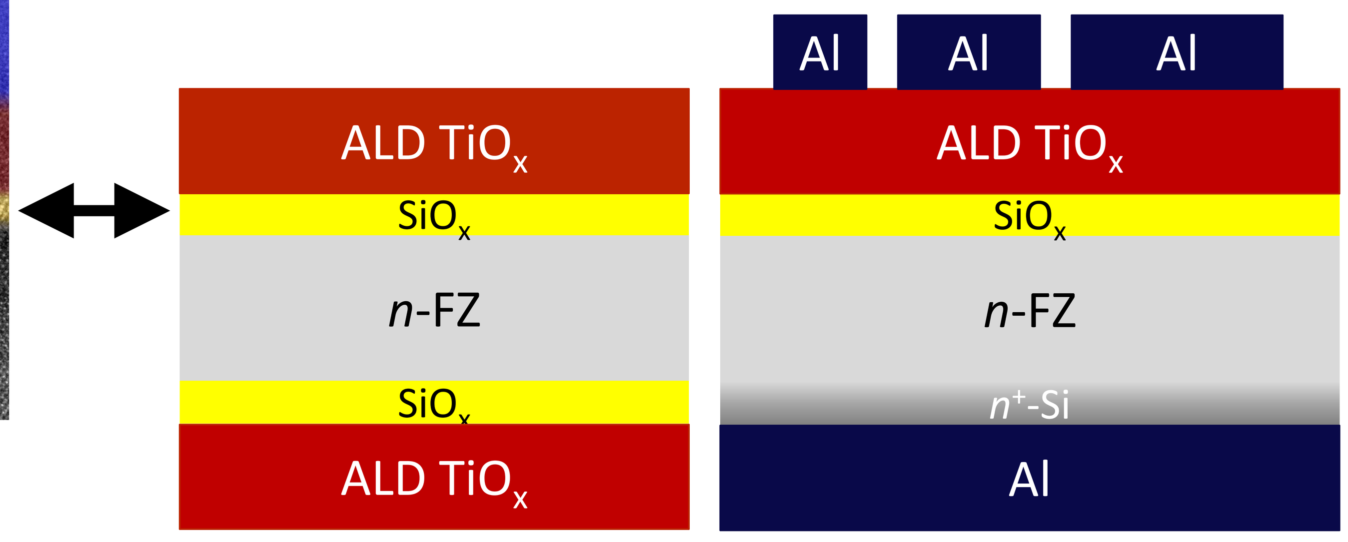


TDMAT



SiO_x formed during ALD TiO_x

Test structures

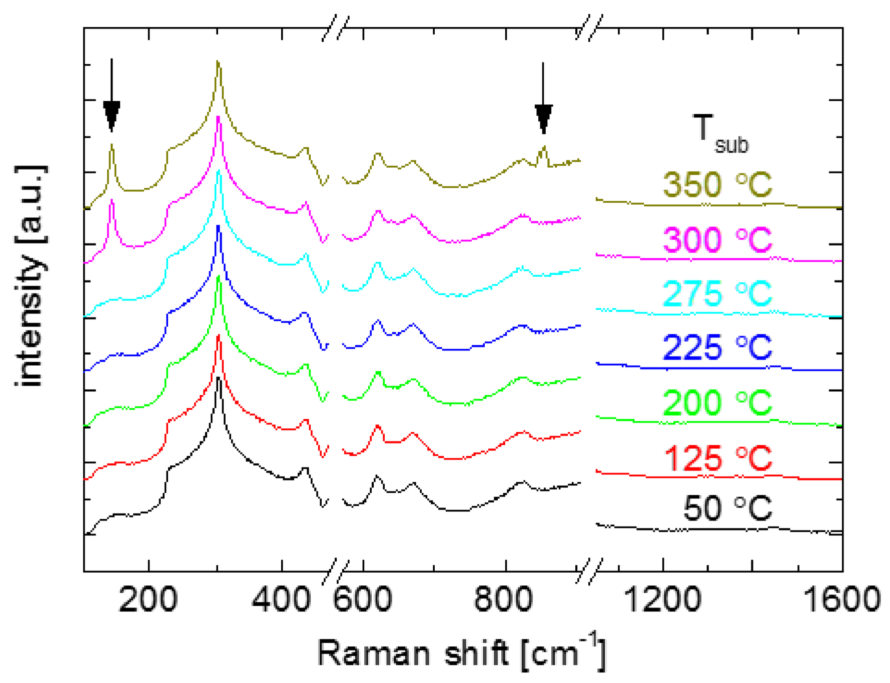


Passivation

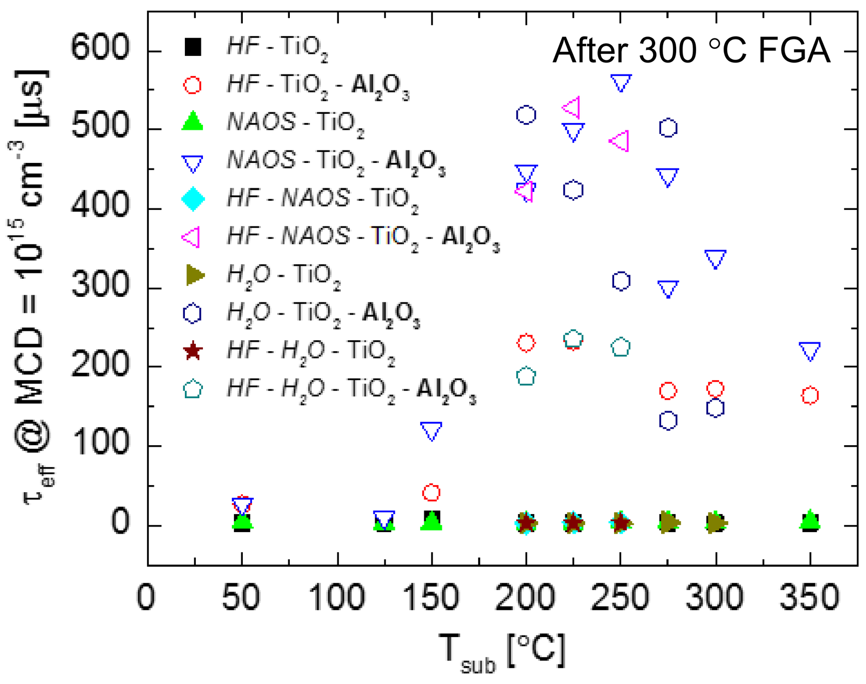
Contact resistivity

Results

O2 plasma ALD $Ti(Cp^{Me})(NMe_2)_3$ (d = 5 nm)



T_{sub} > 300 °C → crystallization



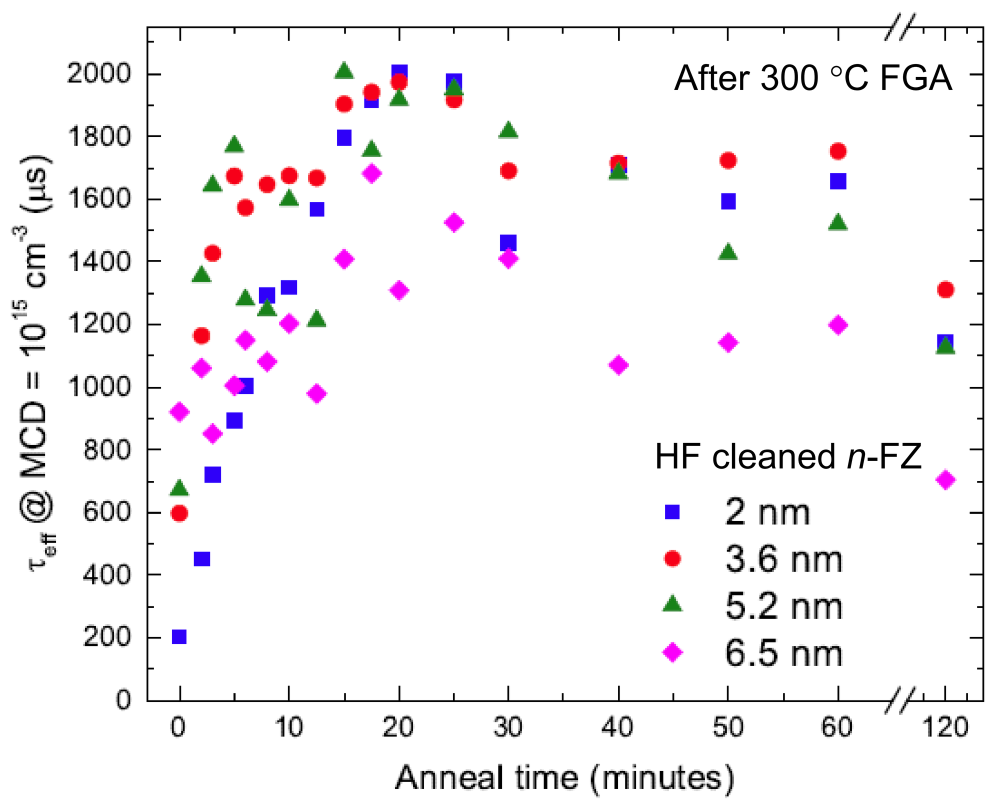
T_{sub} > 300 °C → τ_{eff}↓

FGA / Al_2O_3 / SiO_x variation → τ_{eff} < 600 µs

General TiO_x requirements (for all Ti precursors)

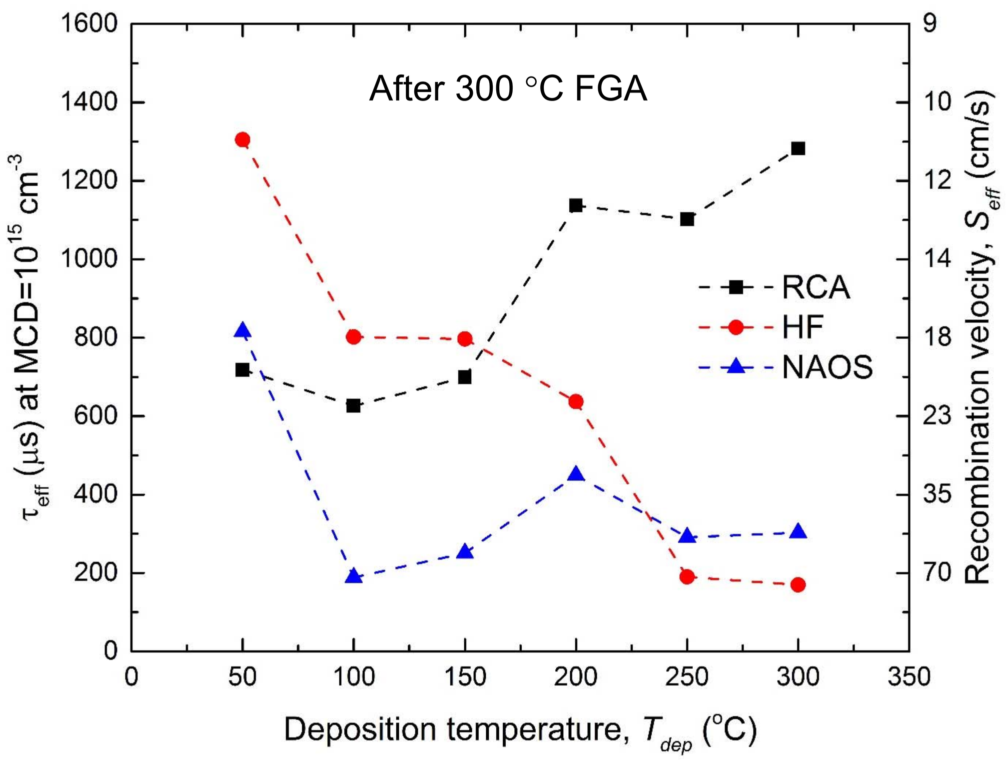
- Amorphous material
- High bandgap (~3.3 eV)
- Thermal ALD to avoid plasma damage (τ_{eff}↓)

Thermal ALD TTIP + H_2O (T_{sub} = 200 °C)

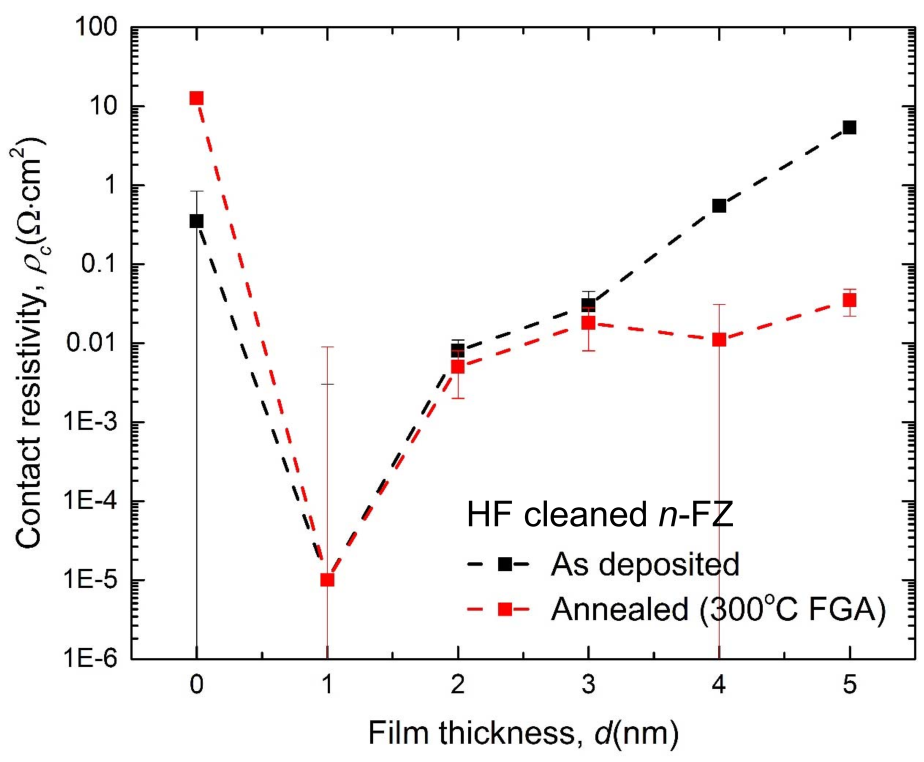


Optimized passivation: τ_{eff} = 2.0 ms
Low growth per cycle (GPC): 0.15 Å
(Plasma ALD TTIP: τ_{eff} < 900 µs)

Thermal ALD TDMAT + H_2O (d = 5 nm)



Good passivation: τ_{eff} = 1.3 ms
Good growth per cycle (GPC): 0.69-0.37 Å
XPS (not shown): HF yields thinnest SiO_x!



Low contact resistivity:
$\rho_{contact} < 10^{-2}$ Ω·cm²

Conclusions

- Passivation: amorphous TiO_x > anatase TiO_x
- Passivation: thermal ALD > plasma ALD
- TTIP: excellent τ_{eff} @ low GPC ☹
- TDMAT: high τ_{eff} & low $\rho_{contact}$ @ good GPC ☺

Outlook

- Test stability in air
- Test stability after metallization
- Sufficient control over band bending in c-Si?[10]
- Preferred solar cell structure for TiO_x contacts?

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