Research Center for Photovoltaics

Ultrathin SiO_x:H / a-Si:H passivation layer for crystalline silicon solar cells

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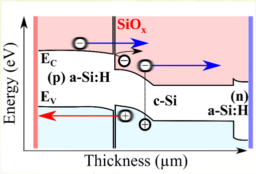
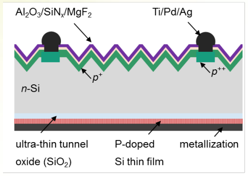
1 – Purpose

- Main objective: **alternative passivation layer** for crystalline silicon solar cells.
- Motivations for **SiO_x material** : potential barrier (**transparent, carrier selective-contacts**), used by notorious **TOPCon structure** [1].



SiO_x for carrier selectivity



TOPCon structure [1]

Challenges: - allowing **tunneling** requires **ultra thin** layer (below **2 nm**).
- keep **high passivation properties**.

- For this, **ALD facility** is used **: precise control** at **atomic scale**.

H atoms directly at interface (**SiO_x:H**) for passivation of **dangling bonds**.

[1] A. Richter et al., *SOLMAT* **173** (2017) 96-105.

2 – Experimental details

Fabrication processes:

- **Wafers**: (n-type) Fz-Si <100>, 280 µm, 1-5 Ωcm.
- **Cleaning**: 4-step chemical process [2].
- **SiO_x or SiO_x:H layers**: deposited by **ALD**.
- **a-Si:H layers**: deposited by **PECVD**.

Characterization techniques:

Quasi Steady-State Photoconductance (**QSSPC**):
✓ Minority carrier lifetime (MCLT) measurement at 1×10^{15} cm^{-3} injection level.

Spectroscopic ellipsometry (SE):
✓ Thickness and bandgap of the films deposited.

Fourier transform infra-red (**FTIR**):
✓ Study of Si-H bindings at wavelength 2000-2100 cm^{-1}.
✓ Si-O bindings at 1050 cm^{-1}.

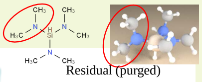
Raman spectroscopy:
✓ Crystallinity of amorphous silicon layers after thermal annealing (TA).

- All these characterizations techniques were performed after **TA temperatures** up to 850°C to underline the evolution of the deposited film properties.

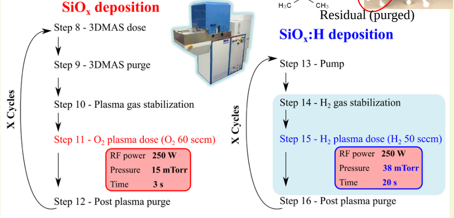
Atomic Layer Deposition (ALD) Process: Oxford Instruments FlexAL system

- Substrate holder: **300°C**
- Spectroscopic ellipsometry **in situ** using **Cauchy Model**
- Inductively Coupled Plasma (ICP) with RF frequency: **13.56 MHz**

- Precursor 3DMAS:
Tris (dimethylamino) silane



Residual (purged)



SiO_x deposition

Step 8 - 3DMAS dose
Step 9 - 3DMAS purge
Step 10 - Plasma gas stabilization
Step 11 - O_2 plasma dose (O_2 60 sccm)

RF power	250 W
Pressure	15 mTorr
Time	3 s

Step 12 - Post plasma purge
X Cycles

SiO_x:H deposition

Step 13 - Pump
Step 14 - H_2 gas stabilization
Step 15 - H_2 plasma dose (H_2 50 sccm)

RF power	250 W
Pressure	38 mTorr
Time	20 s

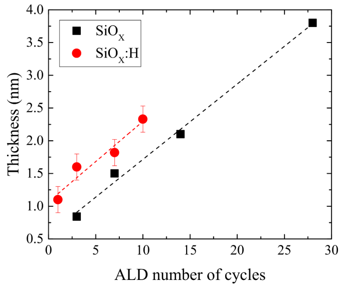
Step 16 - Post plasma purge
X Cycles

Amorphous layer of:
Si / **O** / Si / …

Amorphous layer of:
Si / **O** / **H** / Si / …

[2] S. N. Granata et al., *Energy Procedia* **27** (2012) 412-418.

3 – Thickness control at atomic scale

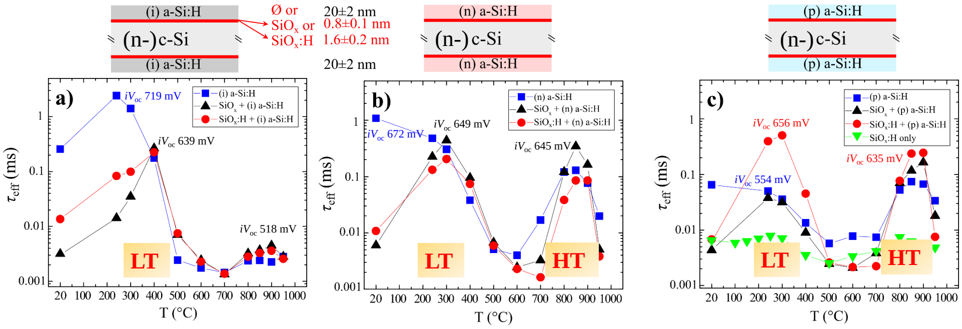


- Precise control of the thickness of SiO_x and SiO_x:H : **linear dependence** with the **number of cycles** during ALD process.

M. Lozac'h et al., *SOLMAT* **185** (2018) 8-15.

4 – Passivation properties of SiO_x and SiO_x:H ultra-thin films

Symmetric structures, wafer: Fz-Si, n-type, 3 Ωcm, 280 µm, oriented ⟨100⟩, double-side polished.



- Passivation at **low-T** (LT), **high-T** (HT) range observable for doped a-Si:H structures. For (p) a-Si:H, **H necessary** for LT.

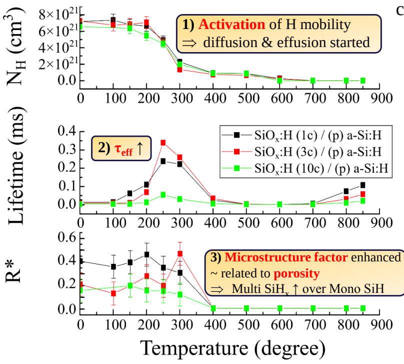
M. Lozac'h et al., *SOLMAT* **185** (2018) 8-15.

5 – Passivation mechanism at low-T for (p)a-Si:H/SiO_x:H stack-layers

Hydrogen concentration, **microstructure factor** calculated from FTIR [3]:

Microstructure factor:

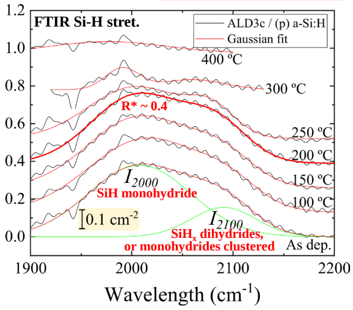
$$R* = \frac{I_{2100cm^{-1}}}{I_{2000cm^{-1}} + I_{2100cm^{-1}}}$$



1) Activation of H mobility
⇒ diffusion & effusion started

2) τ_{eff} ↑

3) Microstructure factor enhanced
~ related to **porosity**
⇒ Multi SiH_x ↑ over Mono SiH

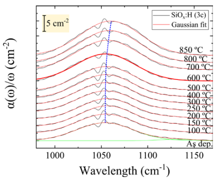


M. Lozac'h et al., *SOLMAT* **185** (2018) 8-15.

[3] A. A. Langford et al., *Phys. Rev. B* **45** (1992) 13367.

6 – Evolution of stoichiometry x with T for SiO_x:H

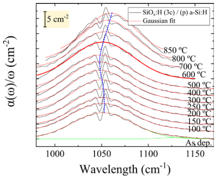
SiO_x:H only

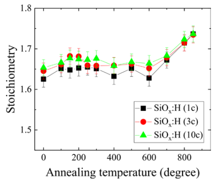


FTIR Si-O stretching ~1050 cm^{-1} [4].

Loss in stoichiometry x at low-T (from 200ºC up to 400ºC) for SiO_x:H /(p)a-Si:H stack-layers (not observed for SiO_x:H only). Followed by improvement of the stoichiometry above 600ºC.

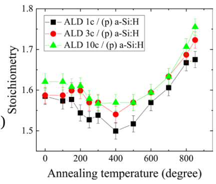
SiO_x:H / (p) a-Si:H





Maximum stoichiometry reaches **1.75**, lower than 2 due to Si substrate.
Note: fully relaxed thermally grown SiO_2 (peak position 1078.5 cm^{-1})

⇒ **Reorganization** at **LT** and **HT**.



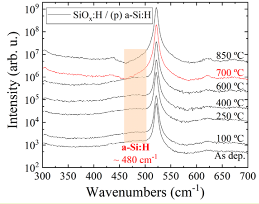
M. Lozac'h et al., *SOLMAT* **185** (2018) 8-15.

[4] E. San Andrés et al., *J. Appl. Phys.* **87** (2000) 1187.

7 – SiO_x:H and SiO_x / (p)a-Si:H passivation at high-T

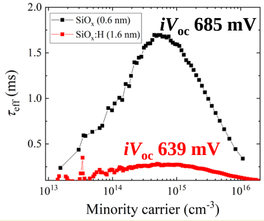
At high-T, SiO_x and SiO_x:H stoichiometries are ~1.75, τ_{eff} is dependent with:

- **SiO_x thickness** (H atoms effused).
- **Doped a-Si:H** (n-, p-) [crystallization occurs above 600ºC (Raman analysis)], and **annealing**.



⇒ **Field effect passivation**: SiO_x (0.6± 0.1 nm) / (p) a-Si:H (17± 1 nm): **τ_{eff}** reaches **1.6 ms** after TA of 850 ºC for 1 h (1 ºC/min).

⇒ Note: thinner SiO_x layer, without H, is beneficial.



8 – Summary and acknowledgments

✓ **Ultra thin SiO_x:H** (< 2 nm) and **SiO_x** (0.6± 0.1 nm) passivation layers were developed by using ALD technique (**atomic scale precision**).
✓ **Low-T (300 ºC)** passivation for SiO_x:H / (p) a-Si:H stack is achieved. **Hydrogenated SiO_x:H** layer greatly enhances the passivation at interface **with (p) a-Si:H** up to 0.5 ms.
✓ At **high-T (850 ºC)**, dopants from **crystallized** a-Si:H induce a **field effect passivation**. SiO_x (0.7 nm) / (p) a-Si:H stack-layers reach **1.6 ms** with an implied V_{oc} of **685 mV**.
✓ Stoichiometry x of SiO_x:H and SiO_x underlines a **reorganization** at low-T and high-T.

Acknowledgments

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