Research Center for Photovoltaics

SiO_x and SiO_x:H grown by ALD as passivation layer for silicon heterojunction solar cells

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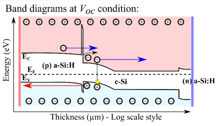
1 – Purpose

- Main objective: provides **alternative passivation layer** for silicon heterojunction (SHJ) solar cells.
- Motivations for **SiO_x material** and **ALD technique**:

1. Large bandgap => **transparent** to solar spectrum.
2. **Carrier selectivity**, h^+ diffusion by **tunneling effect**, repel e^- to reduce recombination inside (p) a-Si:H layer.


Band diagrams at V_{OC} condition:

3. Many ways for deposition:
plasma, UV-O_3, chemical growth HNO_3 H_2O_2, ALD deposition
   - ➢ Precise **control** of thickness at **atomic scale**: **ALD facility**.
4. **Hydrogen** can be easily **incorporated** to form **SiO_x:H** layer.
   - ➢ H atoms can further enhance passivation of **dangling bonds** close to **interface**.

Challenges: - allowing **tunneling** requires **ultra thin** layer (below **20 Å**)
- keep **high passivation properties**

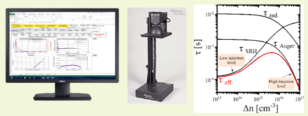
2 – Experimental details

Fabrication process:

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

Effective lifetime measurement:

Quasi Steady-State Photoconductance (**QSSPC**) technique:
☑ Effective lifetime measurement for a broad resistivity range
☑ Measurements at low and high injection levels (Δn : 10^{14} to 10^{17} cm^{-3})
☒ Analysis on the full wafer area only



QSSPC measurement modes:
QSS ⟷ (1/1) **Generalized** (1/64) ⟷ **Transient**

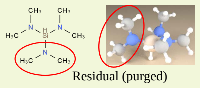
$$\tau = \frac{\Delta n}{G} \quad \text{High injection level} \quad \tau = \frac{\Delta n}{G - \frac{d\Delta n}{dt}} \quad \text{Low injection level} \quad \tau = \frac{-\Delta n}{\frac{d\Delta n}{dt}}$$

Atomic layer Deposition (ALD) Process:

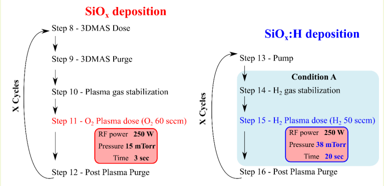
- Substrate holder: **300ºC**
- Spectroscopic ellipsometry **in situ** using **Cauchy Model**
- RF frequency: **13.56 MHz**

➢ Thickness precisely controlled by the **number of cycles**.

- Precursor 3DMAS:
Tris (dimethylamino) silane



Residual (purged)



SiO_x deposition

X Cycles
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 sec**
Step 12 - Post Plasma Purge

SiO_x:H deposition

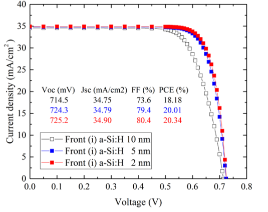
X Cycles
Step 13 - Pump
Condition A
Step 14 - H_2 gas stabilization
Step 15 - H_2 Plasma dose (H_2 50 sccm)
RF power **250 W**
Pressure **38 mTorr**
Time **20 sec**
Step 16 - Post Plasma Purge

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

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

3 – Device simulation

Simulation of the **front** intrinsic **(i) a-Si:H thickness** using AFORS-HET software:


c-Si 300nm, n-type $1.5x10^{16}cm^{-3}$, intrinsic point defects $1x10^{9}$ cm^{-3} (Rear a-Si:H fixed = 10 nm)

Voc (mV)	Jsc (mA/cm2)	FF (%)	PCE (%)
714.5	34.75	73.6	18.18
724.3	34.79	79.4	20.01
725.2	34.90	80.4	20.34

SHJ solar cell structure:

ITO	70 nm
(p) a-Si:H	5 nm
(i) a-Si:H	2~10 nm
c-Si	300 µm
(i) a-Si:H	10 nm
(n) a-Si:H	20 nm
ITO	80 nm
Ag	1 µm
ZnO	20 nm

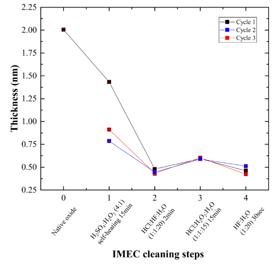
- SHJ solar cell simulated: flat surface & ideal interfaces.

☑ **Thinner (i) a-Si:H layer** at front surface enhances **V_{oc}** and **FF**
- J_{sc} also slightly enhanced (flat surface).

⇒ Underline the importance of this passivation layer to reach **high V_{oc}** and enhanced photo conversion efficiency (PCE).

4 – Thickness control of ultra-thin oxide layer

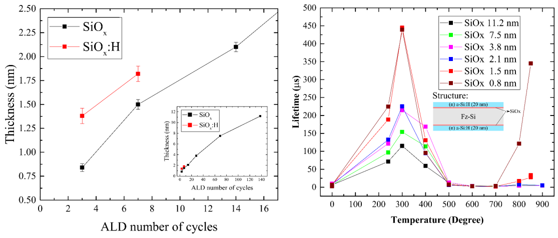
A) Evolution of **oxide layer** during **wafer cleaning** prior to ALD deposition process



☑ Thin layer about 5 Å is observed corresponding to **1 -2 atomic layers** of SiO_x (may grown directly at air ambient).

⇒ Process validates prior to ALD thin films deposition.

B) ALD process: thickness control at atomic scale

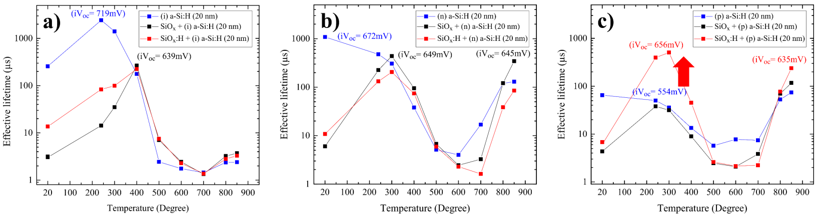


- Precise thickness controlled with number of cycles: 138 cycles ~ **11.2 nm** for SiO_x 3 cycles ~ **8 Å**
- To trigger **tunneling effect**, thickness below 20 Å necessary:
  - ☑ Validate for the three recipes at 7 cycles or below.
  - ⇒ **ALD recipe** with **3 cycles** selected.

☑ After annealing at 300ºC, effective lifetime is enhanced up to 0.45 ms for SiO_x thicknesses below **15 Å**.

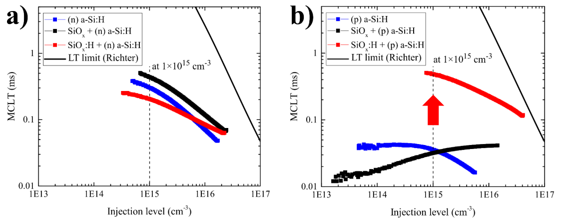
5 – Passivation properties of SiO_x and SiO_x:H ultra-thin films

Symmetric structure **(i) a-Si:H (20 nm)** , **(n) a-Si:H (20 nm)** and **(p) a-Si:H (20 nm):**



- Annealing at **300ºC** and 850ºC improves effective lifetime (MCLT) for (n, p) a-Si:H (Figs. b,c).
  - ☑ Passivation at **low temperature** possible.
- At 300ºC for (n) a-Si:H, SiO_x (8 Å) presents better passivation (Fig. b).
- **Hydrogen incorporation** could improve by one order magnitude MCLT for **(p) a-Si:H** (Fig. c).

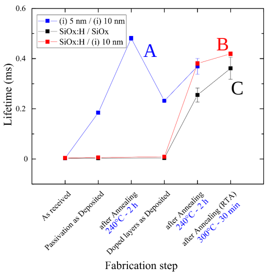
Effective lifetime in function of injection level **at 300ºC**



- Effective lifetime is presented for n-type and p-type a-Si:H (20 nm) with SiO_x (black), SiO_x:H (red) and without (blue).

☑ Effective lifetime is enhanced by **one order of magnitude** by using hydrogenated **SiO_x:H** passivation films at interface with **(p) a-Si:H layer**.

6 – Evolution of lifetime with SHJ fabrication process



Structure A

ITO	70 nm
(p) a-Si:H	5 nm
(i) a-Si:H	5 nm
c-Si	300 µm
(i) a-Si:H	10 nm
(n) a-Si:H	20 nm
ITO	80 nm
Ag	1 µm
ZnO	20 nm

Structure B

ITO	70 nm
(p) a-Si:H	5 nm
	13.8 Å SiO_x:H
c-Si	300 µm
(i) a-Si:H	10 nm
(n) a-Si:H	20 nm
ITO	80 nm
Ag	1 µm
ZnO	20 nm

Structure C

ITO	70 nm
(p) a-Si:H	5 nm
	13.8 Å SiO_x:H
c-Si	300 µm
	8 Å SiO_x
(n) a-Si:H	20 nm
ITO	80 nm
Ag	1 µm
ZnO	20 nm

⇒ During fabrication process, effective lifetimes of structure B and C are of the **same order as structure A (5 nm a-Si:H front)**, about 0.4 ms **after annealing** at 300ºC for 30 min.

7 – Conclusion and acknowledgments

☑ **Ultra thin** layers **SiO_x:H** (14±1 Å) and **SiO_x** (8±1 Å) with high reproducibility deposited by ALD technique were developed.
☑ Fabrication process at **low temperature (300ºC)** possible.
☑ **Hydrogenated SiO_x:H** layer greatly enhances the passivation at interface **with (p) a-Si:H**.
☑ During SHJ solar cell fabrication process: **Effective lifetime** about 0.4 ms **similar to intrinsic a-Si:H with 5 nm thick** at front and 10 nm thick at rear.

Acknowledgments

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