Self Assembled Monolayers for Passivated Contacts

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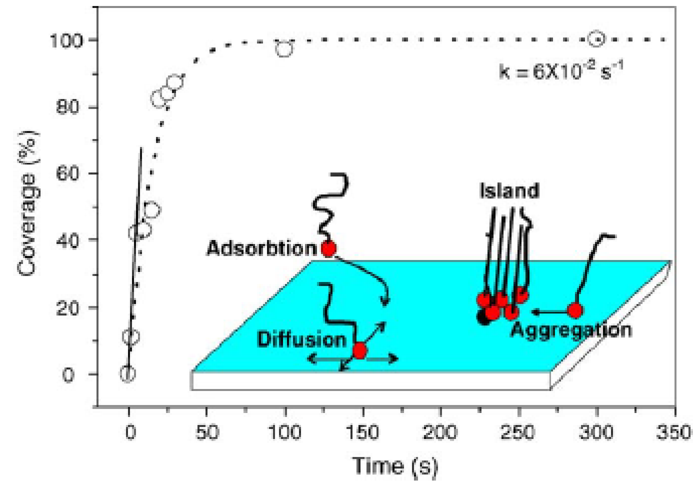
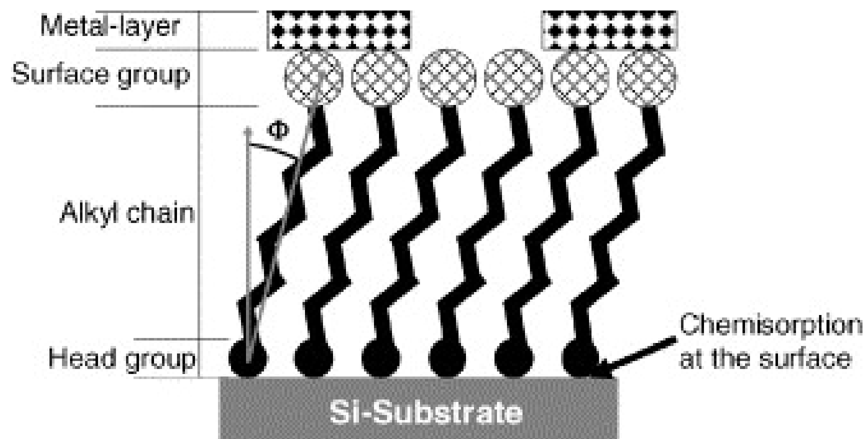
Motivation to Improve Passivated Contact Solar Cells

- Poly-Si on SiO_2 Passivated Contacts
  - Blistering/Adhesion of Poly-Si
  - Engineer Interfaces to Tailor Doping
- Lithography is Expensive and Time Consuming
  - Photoresist Free Patterning
- Self Assembled Monolayers (SAM)
  - Inexpensive
  - Can be Applied in Batch Processes

Self Assembled Monolayer (SAM): Background

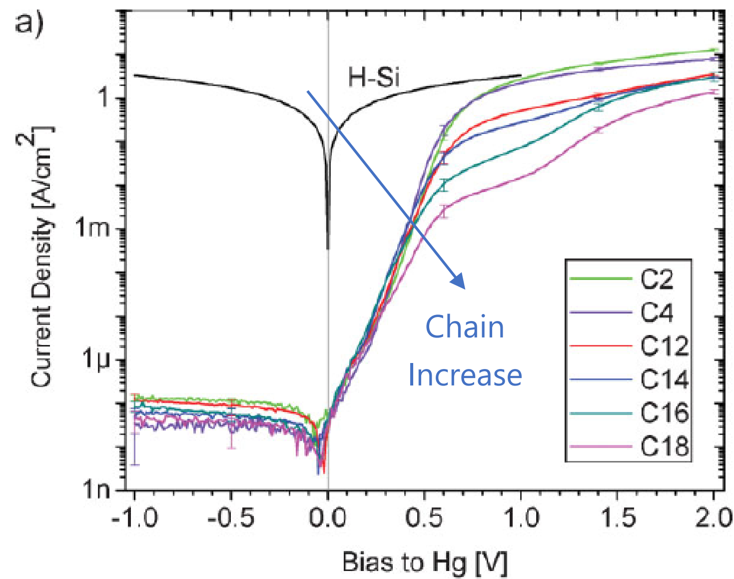
SAM Precursor + Substrate Surface Govern Attached Chemistry





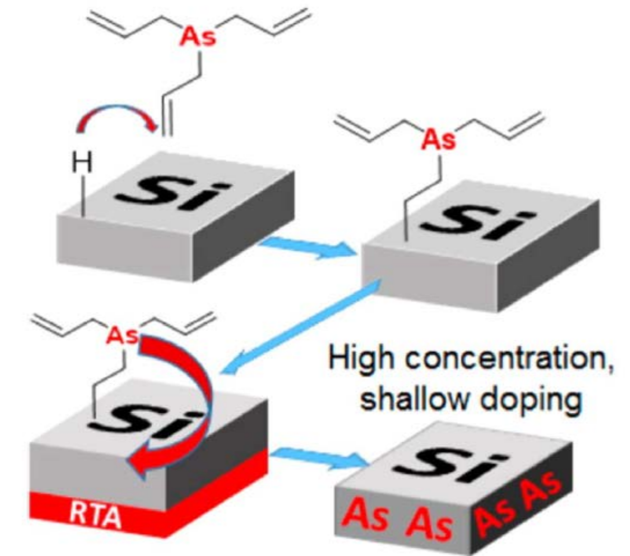
Aswal, et al. An. Chim. Acta. 568, (2006) 84.

Chain Length Increases Dielectric Thickness



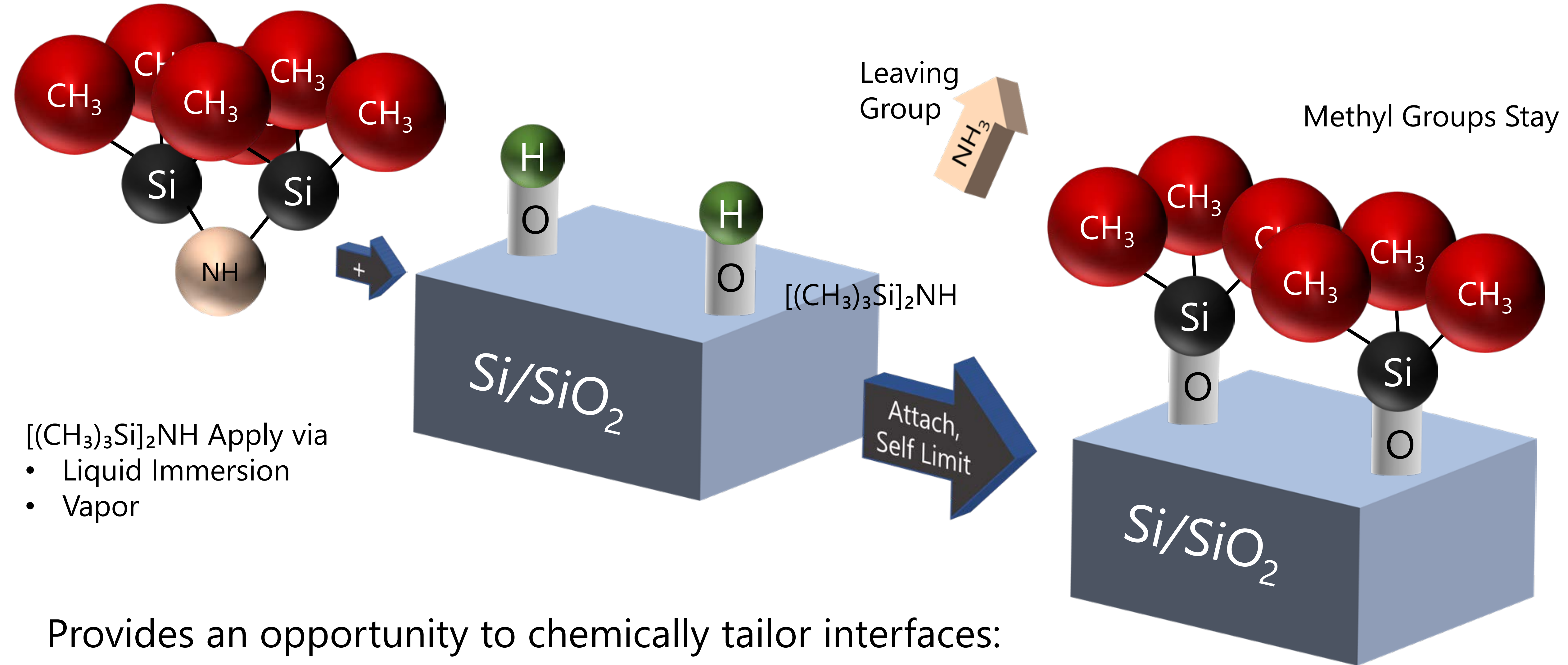
Vilan, et al. Adv. Mater. 22, (2010) 140.

Monolayer Doping Capability



Ye, et al. Mat. Sci. Semic. Proc. 62, (2017) 128.

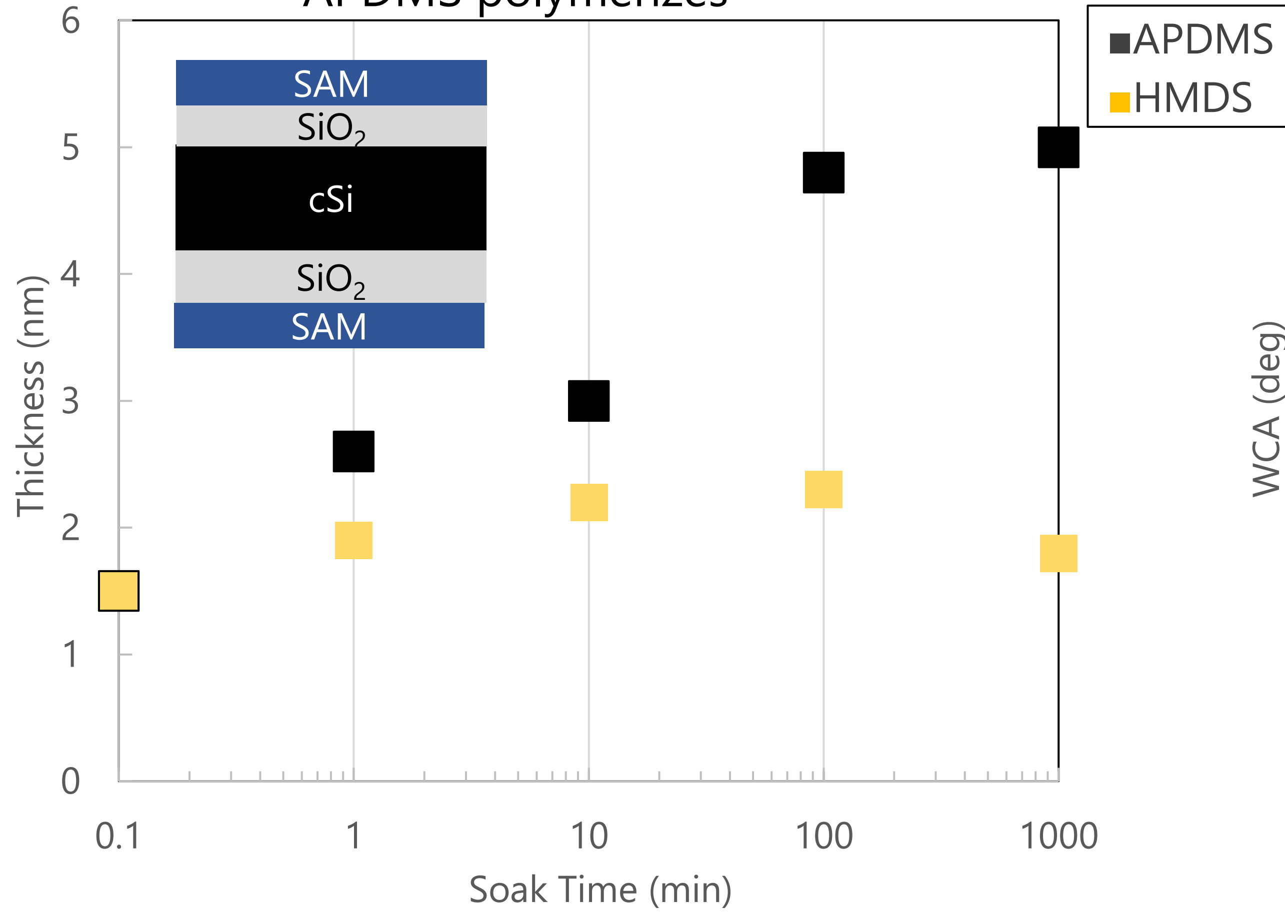
Hexamethyldisilazane (HMDS) Functionalization



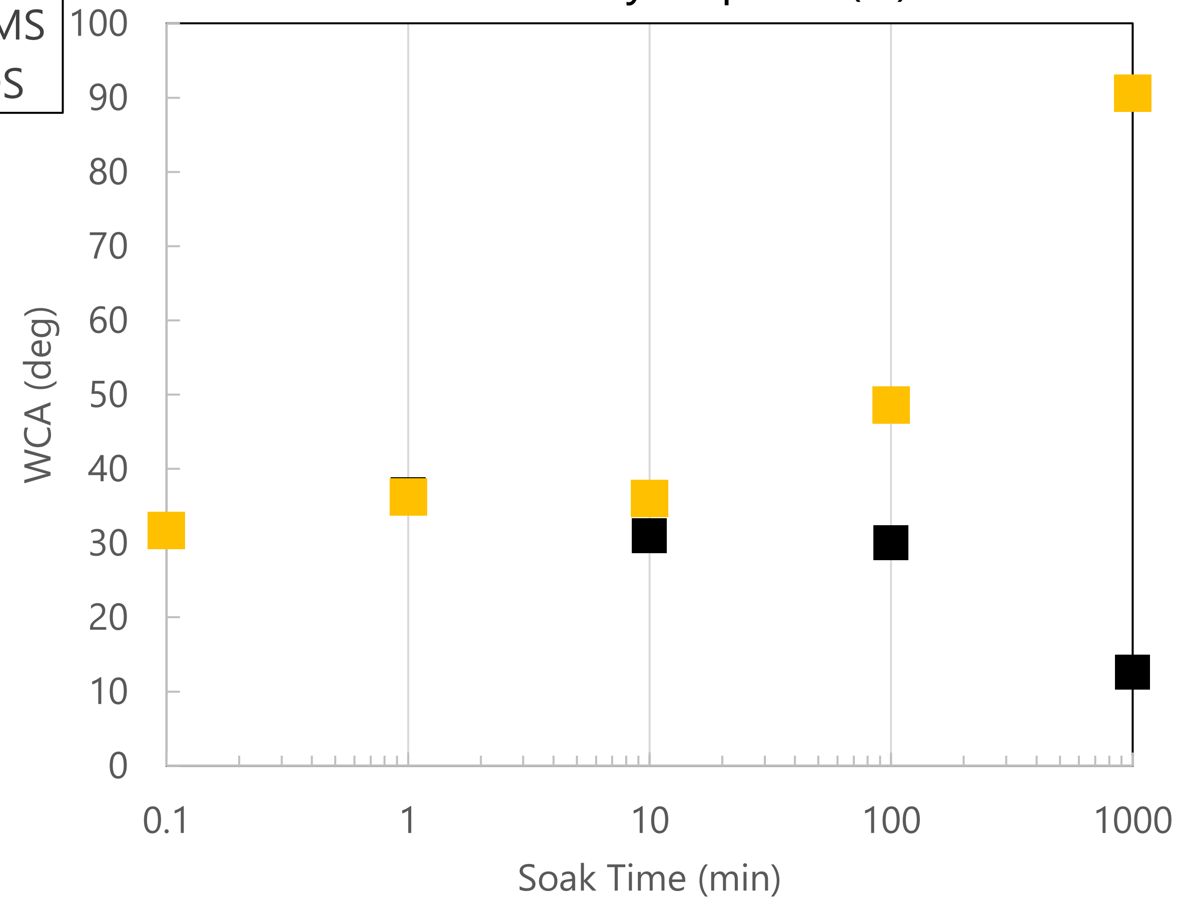
Provides an opportunity to chemically tailor interfaces:
-Add carbon in this case

HMDS vs Aminopropyldiethoxymethylsilane (APDMS)

Ellipsometry
- HMDS self terminates
- APDMS polymerizes



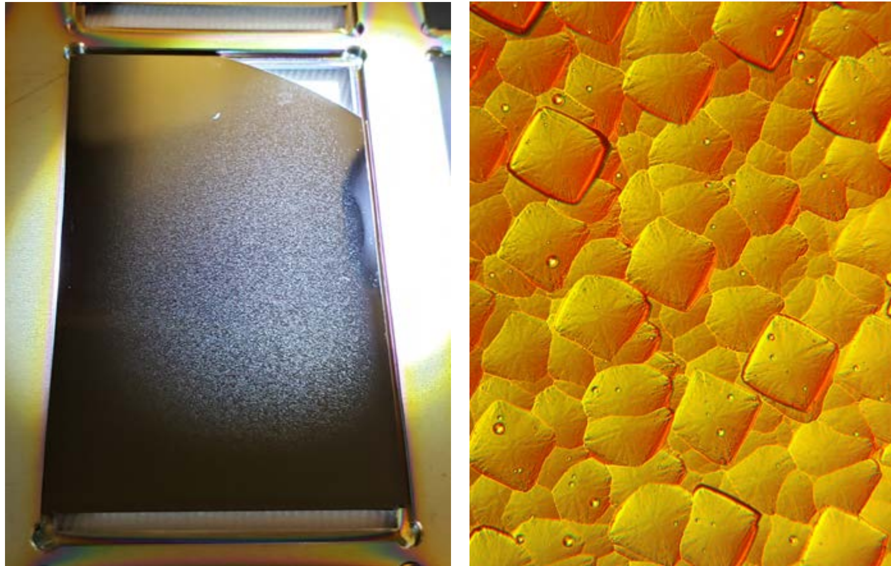
Water Contact Angle↑ Surface Coverage↑
- HMDS surface coverage increases with time
- APDMS remains hydrophilic (N)



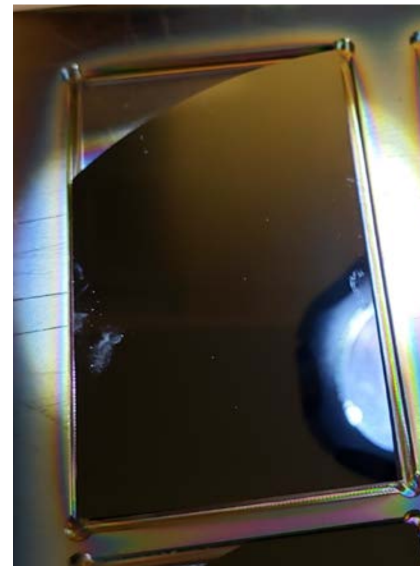
Hexamethyldisilazane (HMDS) Blister Mitigation

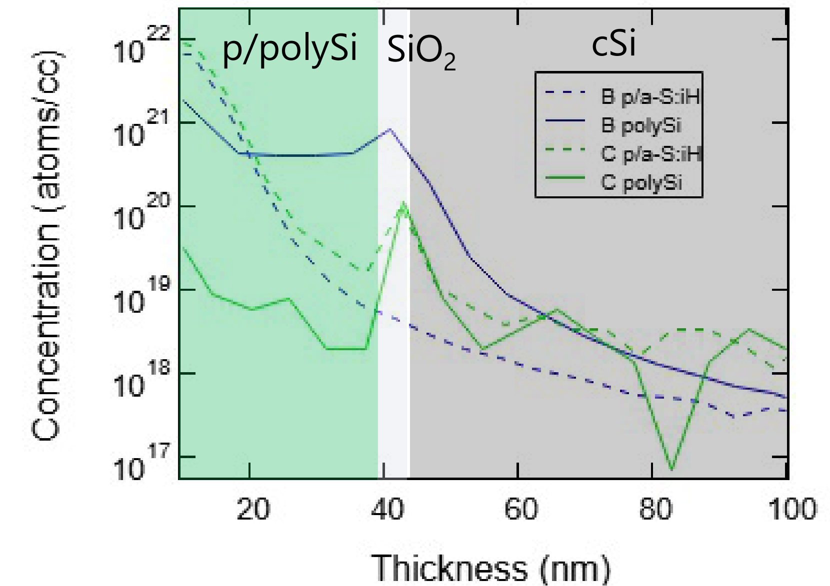
$[(CH_3)_3Si]_2NH$

No HMDS – Blistered



HMDS - Promoted Adhesion





- p/a-Si:H most likely to blister: Lower H effusion temperature
- C added to a-Si:H helps prevent blistering
  - Nogay, et al. *IEEE J. Phot.* 8.6 (2018): 1478-1485.

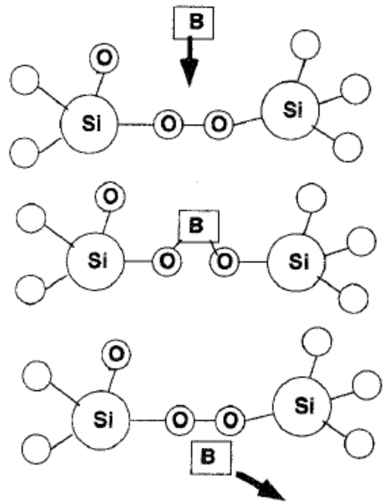
Isolate p/poly-Si to SiO_2 Interface for Devices

n/aSiH
nCz
SiO_2

n/aSiH
nCz
SAM

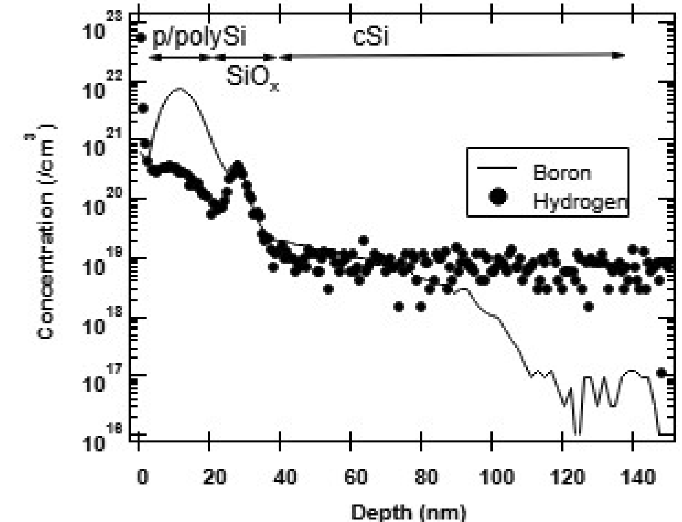
n/aSiH
nCz
i/aSiH
p/aSiH

Grid
SiNx
n/polySi
nCz
i
p/polySi
i
Metal



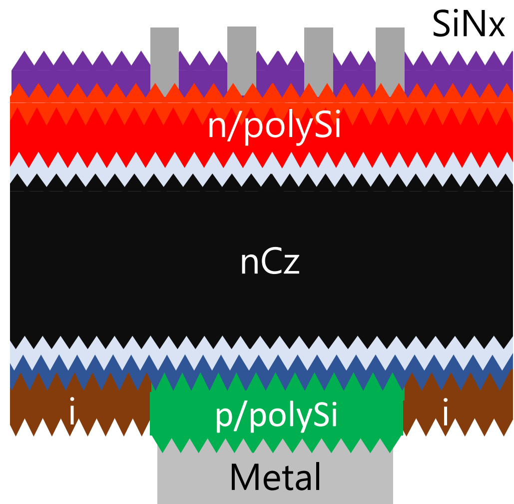
Mitigate Boron:

- Defect in SiO_2
  - (Peroxy Linkage Defect)
- High cSi B surface concentration
- B pile-up at SiO_2 interface

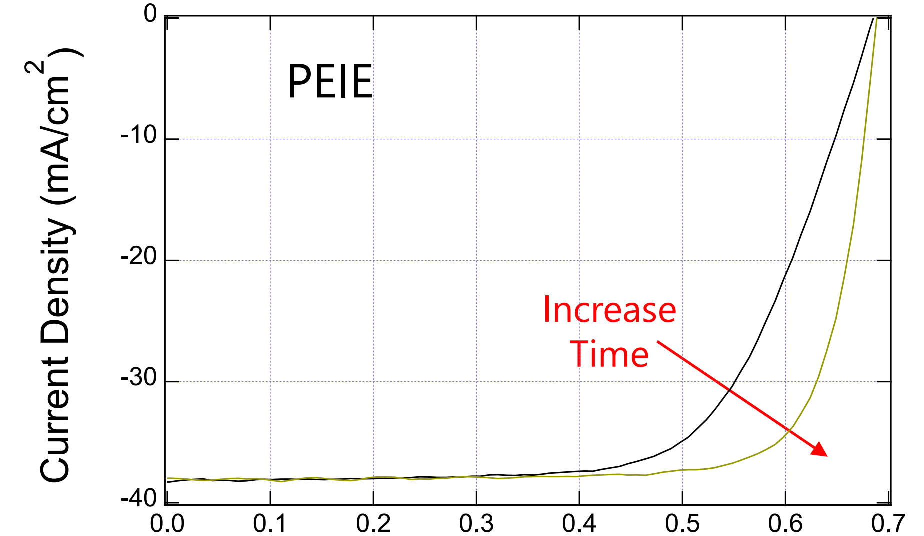


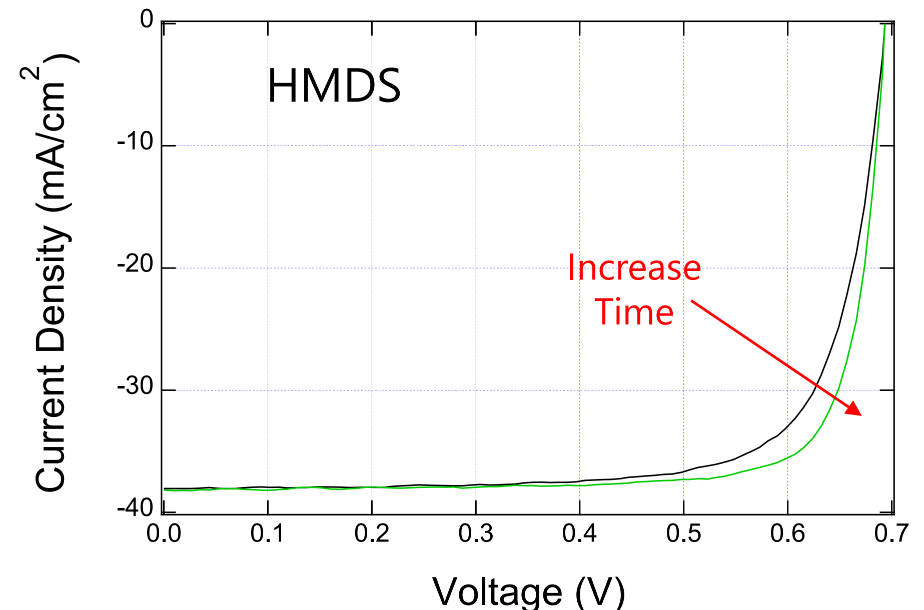
Fair. *IEEE Elect. Dev. Lett.* 17.5 (1996): 242.

Extended Crystallization Time Improves Fill Factor



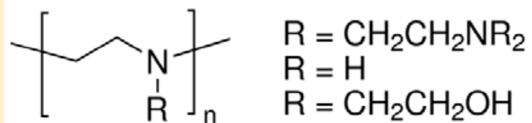
SAM	850°C time (min)	iV_{oc} (V)	V_{oc} (mV)	J_{sc} (mA/cm^2)	FF	η (%)
PEIE	30	0.700	686	38.2	**66.7**	17.5
	30	0.704	685	38.3	**68.1**	17.9
	30	0.701	690	38.0	**75.4**	19.8
	160	0.698	690	38.0	**78.9**	20.7
	160	0.702	690	38.7	**76.1**	20.3
	160	0.702	691	38.0	**76.9**	20.2
HMDS	30	0.701	700	38.0	**76.4**	20.3
	30	0.700	695	38.1	**75.3**	19.9
	30	0.700	701	38.4	**77.2**	20.8
	160	0.698	691	37.8	**79.5**	20.8
	160	0.701	695	38.0	**78.6**	20.8
	160	0.699	696	38.2	**80.4**	21.4





<u>PEIE – no Si</u>

Polyethylenimine Ethoxylated



www.sigmaaldrich.com

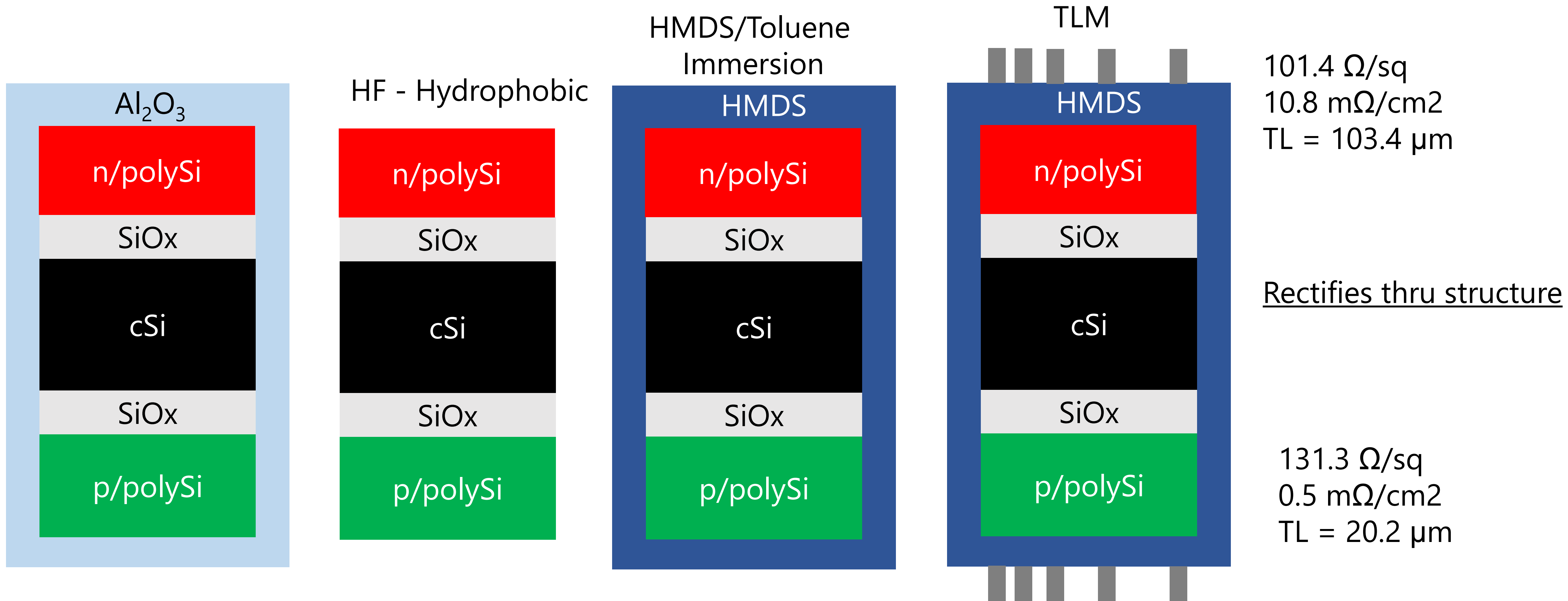
<u>HMDS</u>

$[(CH_3)_3\mathbf{Si}]_2NH$

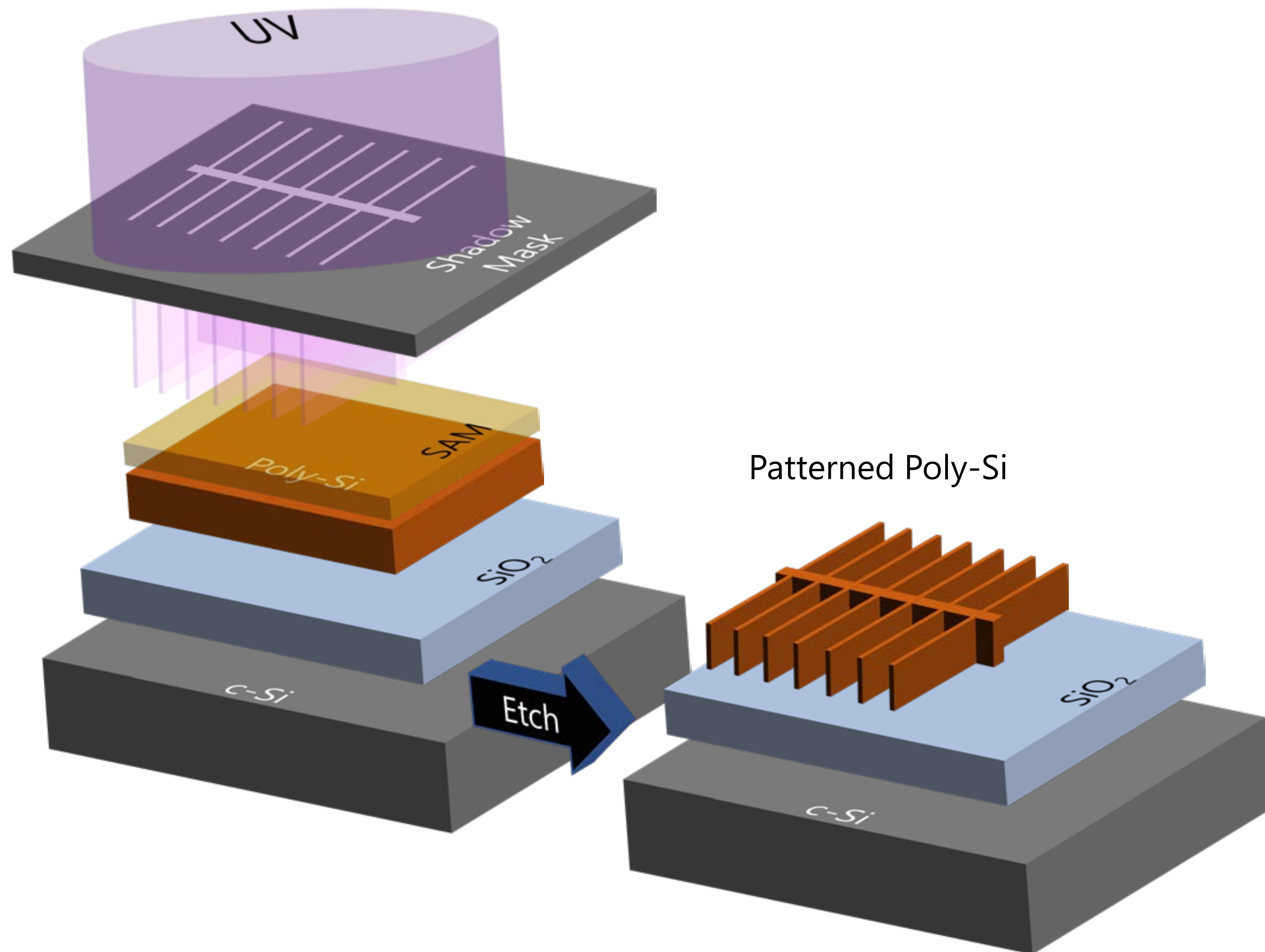
Longer 850°C Anneal

- Carrier collection improved
- Maintain passivation
- Increased dopant diffusion
- SAM dielectric thickness decreased

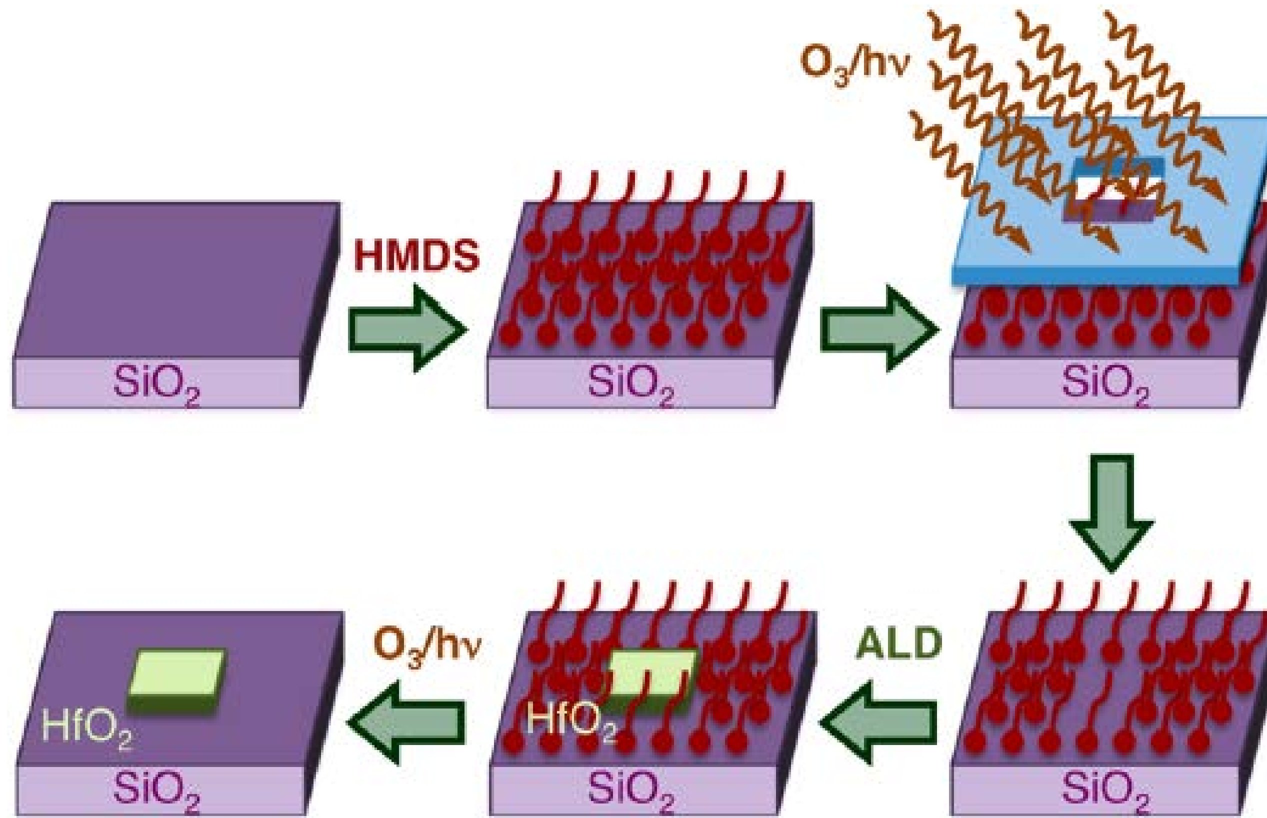
Metallization on HMDS: Allows Transport SAM Removal Unnecessary

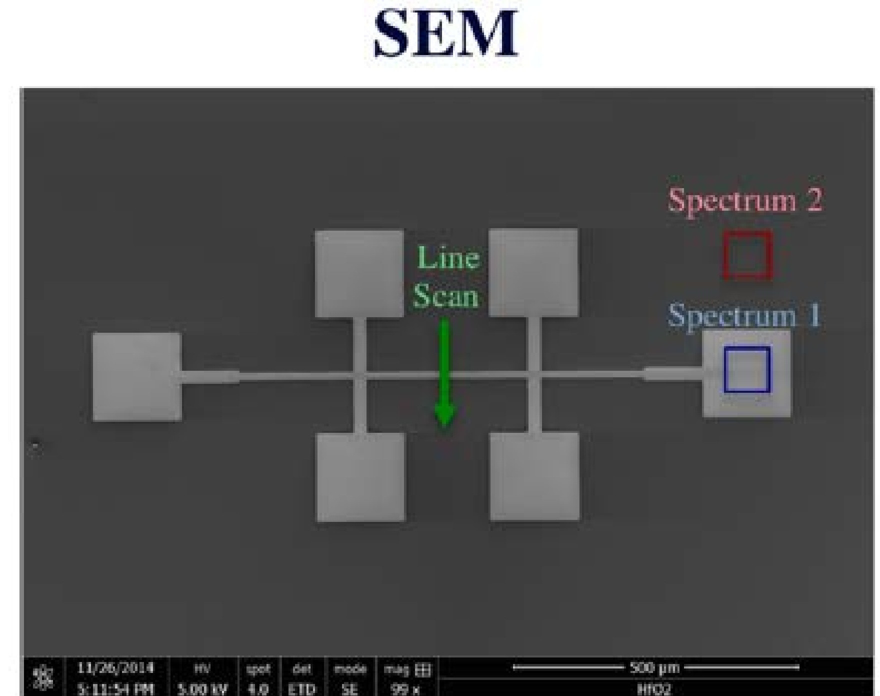


Different Application for SAM Application
Patterning Solar Cell Layers – Photoresist Free Lithography



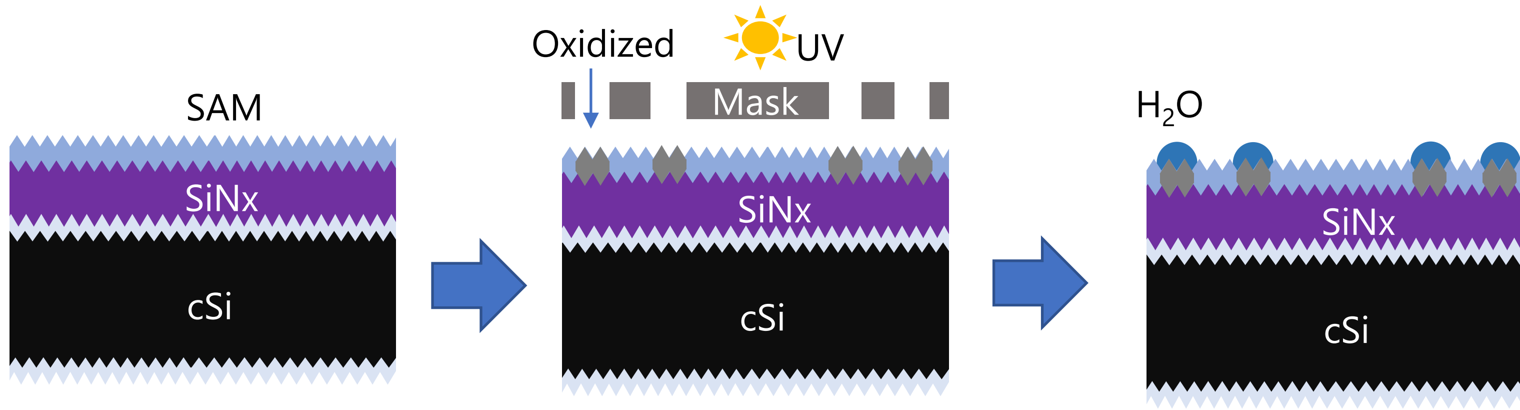
Patterning with HMDS Background – Selective ALD



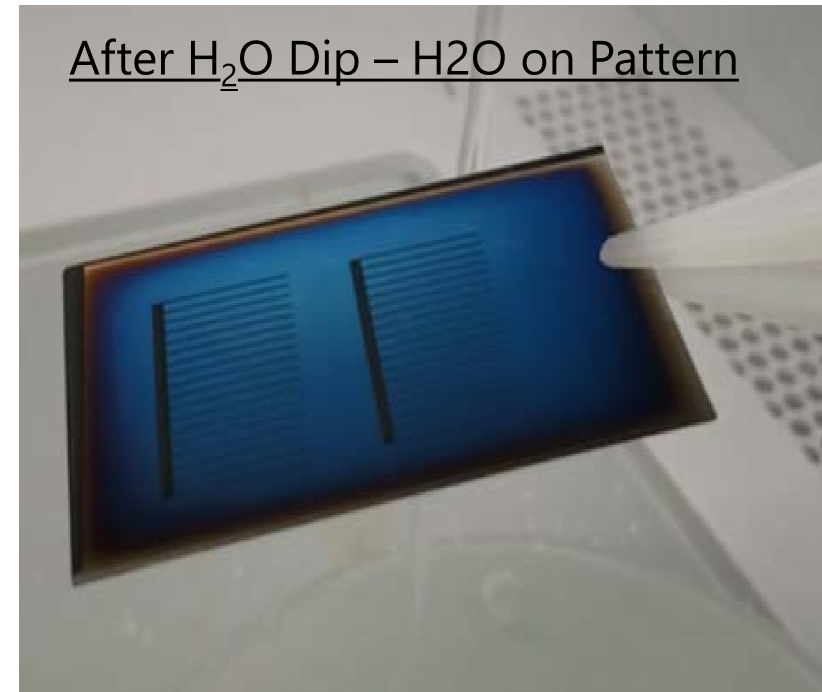


Guo, et al. *ACS applied materials & interfaces* 8.30 (2016): 19836.

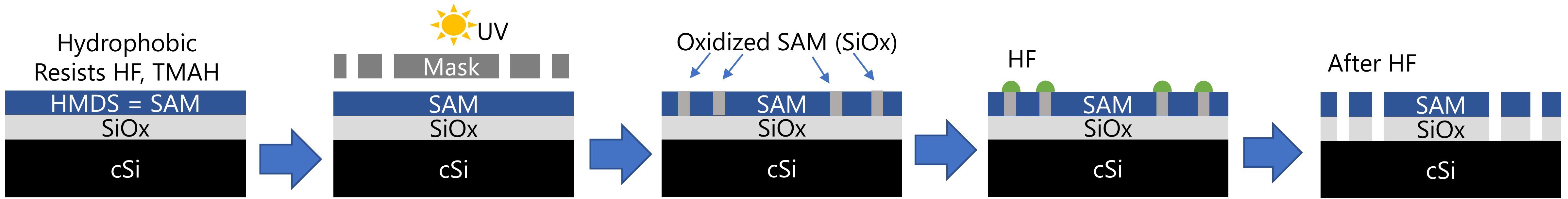
HMDS Pattern with UV – Water Adheres to Oxidized Pattern



- Oxidized SAM is Hydrophilic
  - UV photocleaves organic groups
    - Calvert, et al. Thin Solid Films, 210 (1992) 359.
- SAM (HMDS) is Hydrophobic



HMDS Patterned Selective Etching cSi

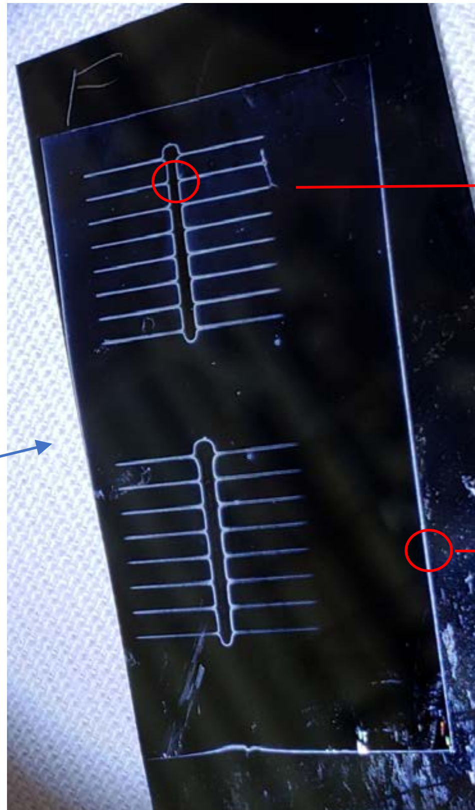


After TMAH

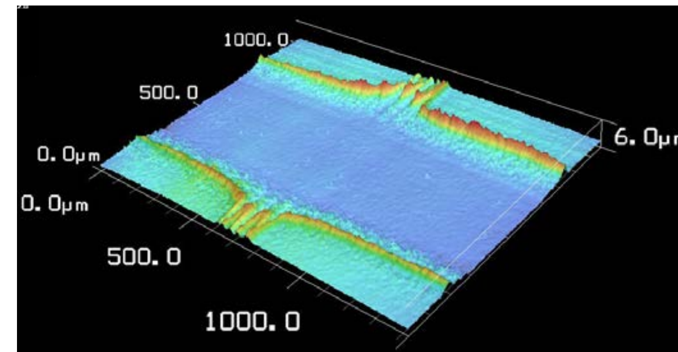
SAM
SiOx
cSi

Grid Pattern Etched after TMAH Soak

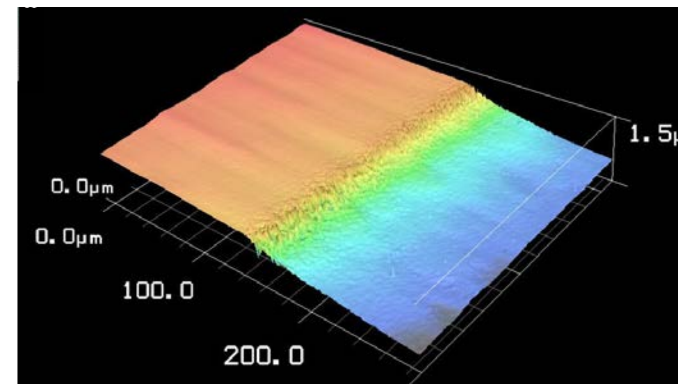
Rectangle = Mask



Etched Busbar



SAM protects cSi from TMAH



HMDS Reversed Patterned Etching a-Si:H – No HF

UV time

Mask

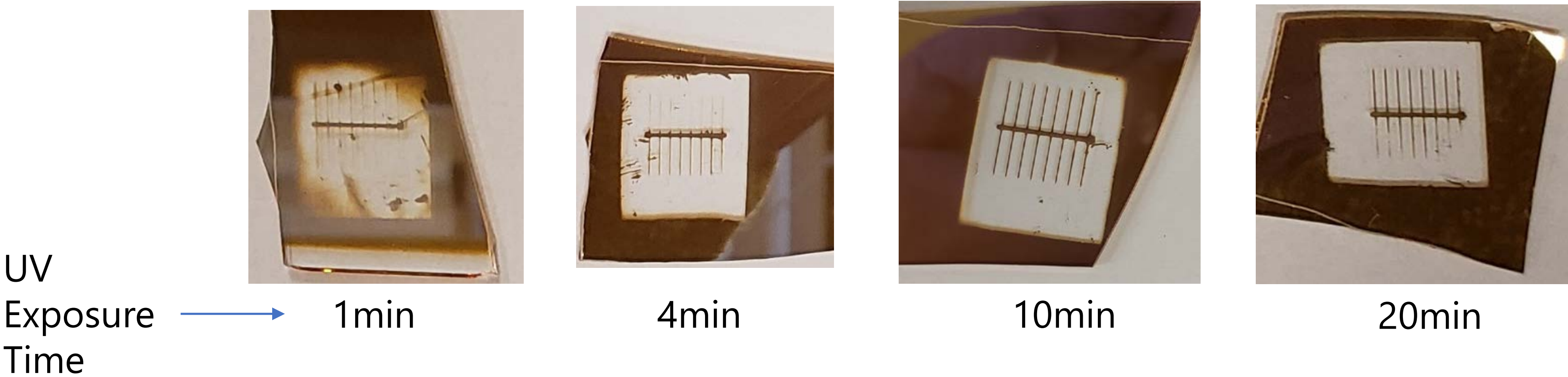
SiOx

±HMDS

i/aSiH

Glass

TMAH



Oxidized HMDS
- Resists TMAH

No HMDS
- Oxidized a-Si:H
- Does not resist TMAH

Inverse SAM Patterned Etching a-Si:H on SiO_2

HMDS
a-Si:H
SiO_2
nCz

UV Through Mask
Oxidizes HMDS

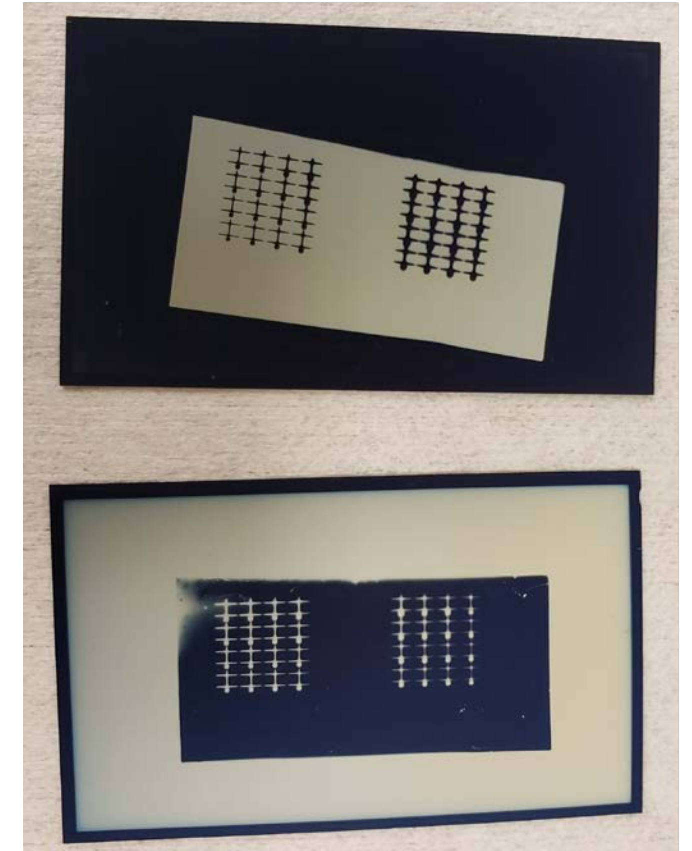
SiO_2 HMDS

HF

No HF

HMDS Blocks TMAH

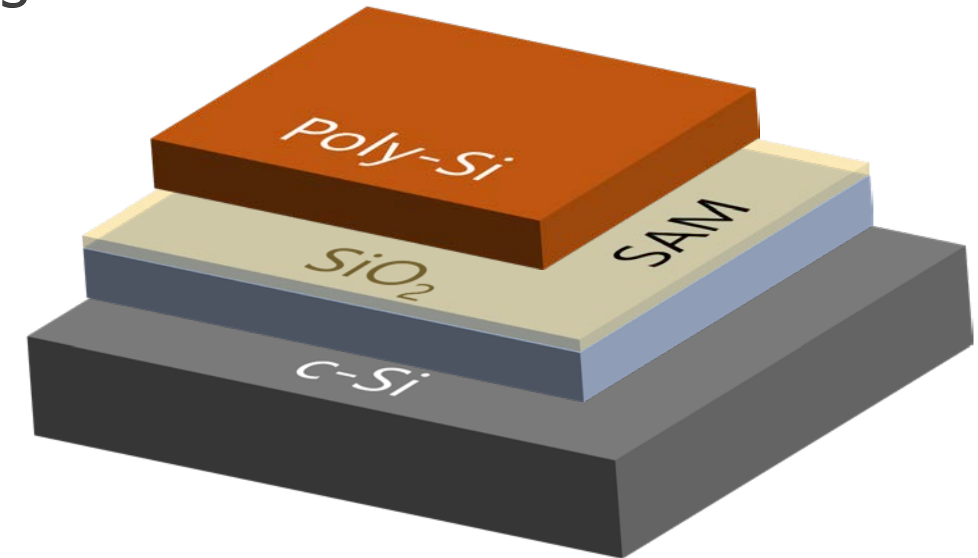
SiO_2 Blocks TMAH



Conclusions

SAMs offer multiple prospective applications

- Engineered interfaces
- Selective doping
- Metallization schemes
- Poly-Si removal between grid fingers



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