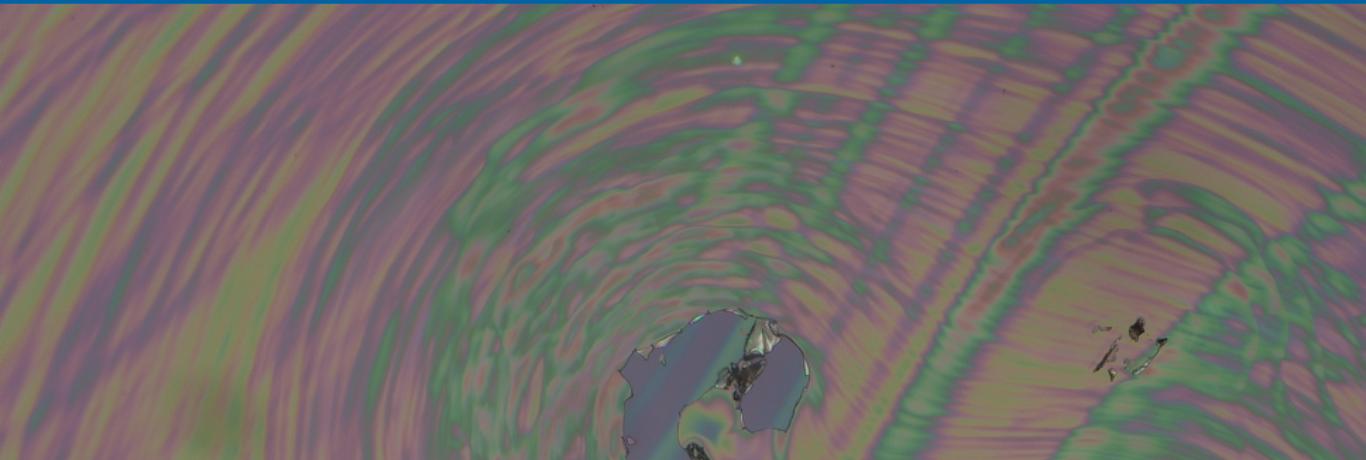
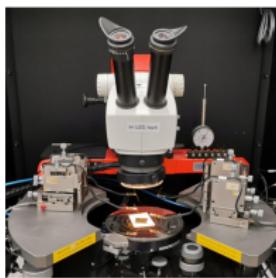
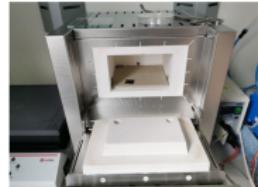


# Particle Swarm Optimization for Electrical Passivation of Steel Substrate Using Zirconium Oxide

PSO for Steel Passivation with ZrO





## Thin-Film Photovoltaics: CIGS modules

- high absorption coefficient
- connected in series
- substrate:
  - must be insulating
  - mostly glass



# Adaption of Precursor Solutions Recipe

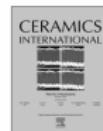
Ceramics International 42 (2016) 16867–16871



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A new sol-gel route to prepare dense Al<sub>2</sub>O<sub>3</sub> thin films

Baofu Hu\*, Erguang Jia, Baoli Du, Yuehong Yin\*

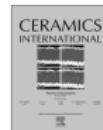


# Adaption of Precursor Solutions Recipe

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recipe	original	adapted
solvent	EtOEt	BuOH
precursor	Al(OPr <sup>i</sup> ) <sub>3</sub>	Zr(OPr) <sub>4</sub>
chelating agent	AcAc	AcAc
stabilizing agent	AcOH	iPrOH/AcOH

# Different Precursor Concentrations

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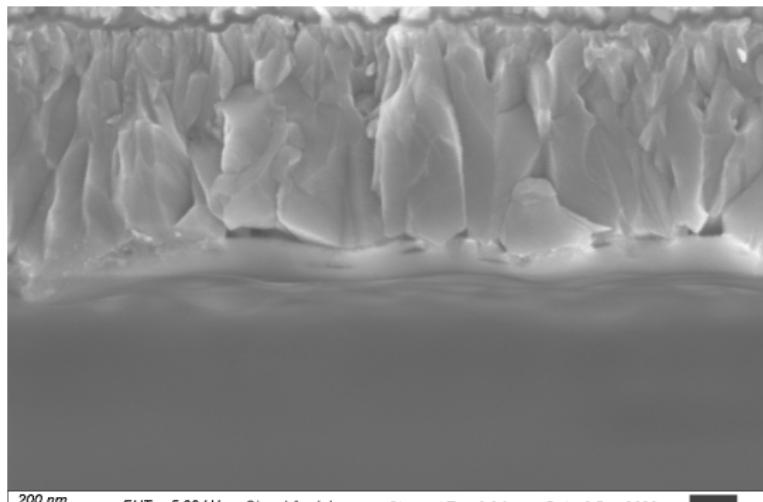
	1x	2x	3x	4x	5x
BuOH [ml]	4.95	4.9	4.85	4.8	4.75
ZrPro [ml]	0.05	0.1	0.15	0.2	0.25
AcAc [ml]	0.0125	0.025	0.0375	0.05	0.0625
IPO/AcOH [ml]	2	2	2	2	2

## Tape Casting and Calcination

- Tape Casting
  - temperature: 40-80°C
  - blade speed: 10-20mm/s
- Calcination
  - temperature: 300-500°C
  - heating rate: 2-18°C/min



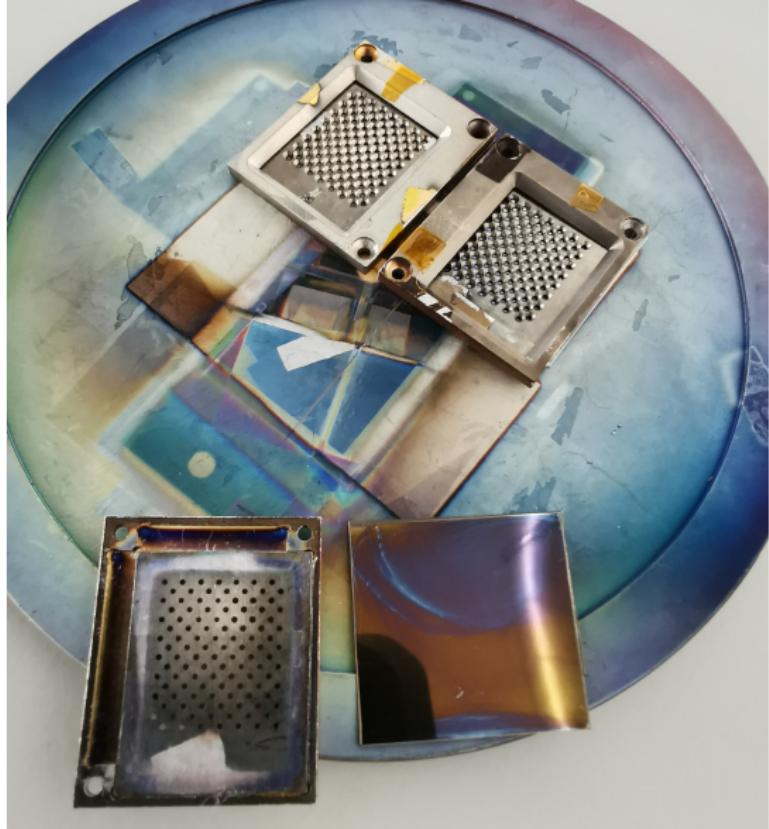
## Cross Section of $\text{ZrO}_2$



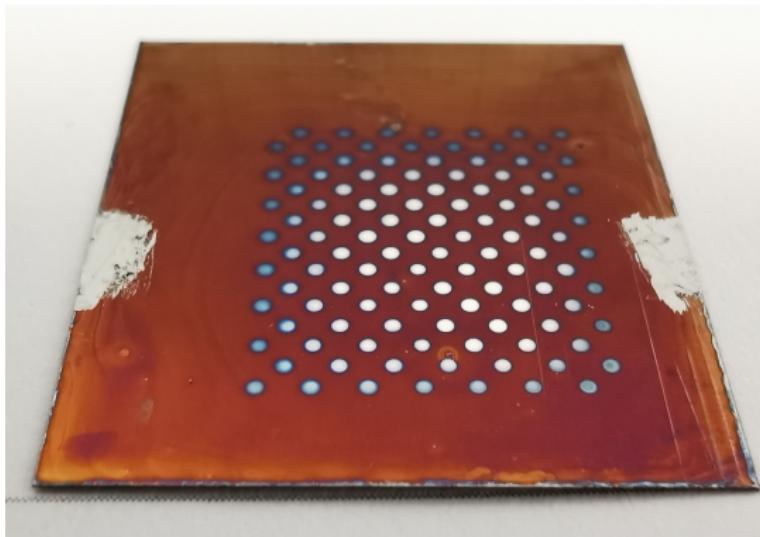
- Scanning Electron Microscope
- substrate: FTO (Fluorine Doped Tin Oxide)
- single layer of  $\text{ZrO}_2$

## Application of Contacts

- Bottom left: Shadow mask
- Bottom right: Steel substrate  $\text{ZrO}_2$  layer
- Top: samples with mask attached



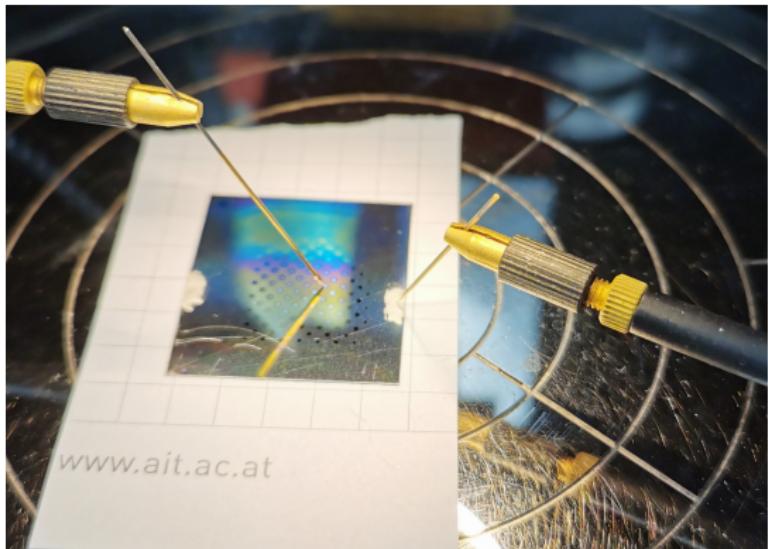
## Applied Contacts



- passivated sample with array of contacts
- contacts to steel on edges

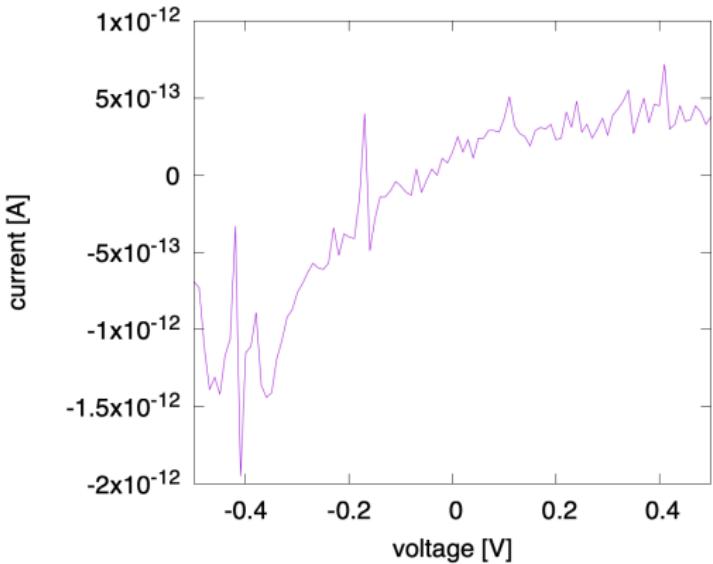
## Measuring Current Voltage Characteristics

- left needle touches top contact ( $\text{ZrO}_2$ )
- right needle touches bottom contact (steel)



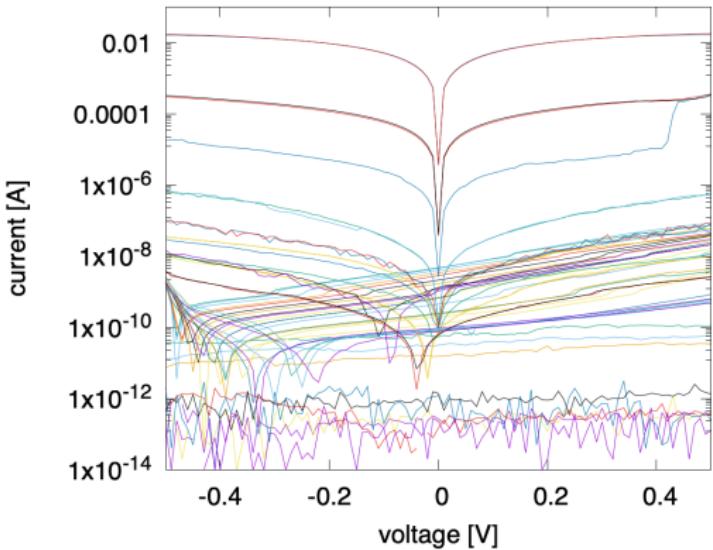
## Current-Voltage characteristics

- voltage sweep
- 10mV steps
- very low current
- low conductivity
- high resistance



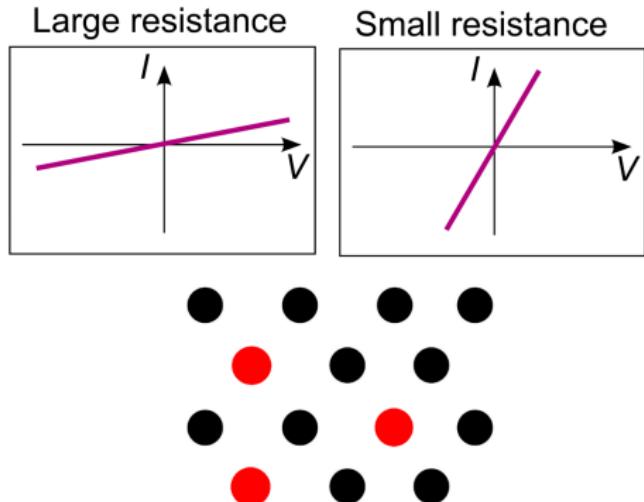
## Current-Voltage characteristics II

- all measurements of single sample
- huge range
- low current
- high current



## Pin Hole Density and Leakage Current

- Conductivity
  - $g = \frac{dI}{dV} \Big|_{V=0}$
- Pin Hole Density
  - $s_i = \begin{cases} 1 & \text{if } g_i < 10^{-5} \\ 0 & \text{if } g_i \geq 10^{-5} \end{cases}$
  - $\rho = \sum_i^N \frac{s_i}{N}$
- Leakage Current
  - $\gamma = \sum_i^N \frac{(-\log_{10}(g_i) - 13)^2}{N}$



## Particle Swarm Optimisation



- inspired by fish schools
- iterative process
- particles:
  - input vars: position
  - velocity
- next times step
- R package `emma`

## Input Variables for Optimisation

- precursor solution concentration
- number of layers
- coating temperature
- blade speed
- calcination temperature
- calcination heating rate

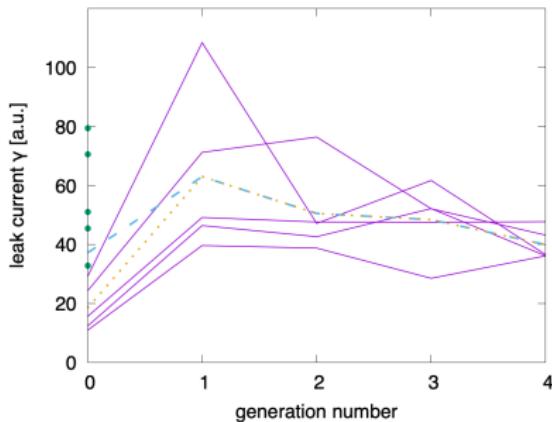
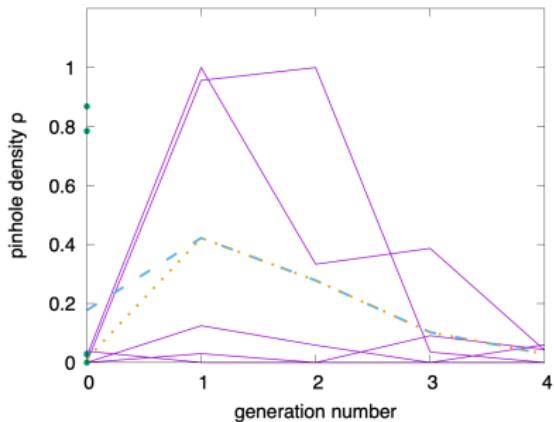
## Input Variables for Optimisation

$c_{zr}$ [22mmol/L]	$n_L$	$T_C$ [°C]	$v_C$ [mm/s]	$T_{cal}$ [°C]	$v_{cal}$ [°C/min]
2	4	40	10	300	2
3	6	50	12	400	6
4	8	60	14	500	10
5	10	70	16		14
	12	80	18		18
			20		

Table: Discrete levels of each input parameter

## Particle Swarm Optimisation Iterations

- metrics are reduced per generation
- model learned to represent data



## Summary

- found recipe for dense  $\text{ZrO}_2$  via sol-gel
- prepared insulating  $\text{ZrO}_2$  layers
- optimization chose correct input variables