Sol-gel ZrO_2 film optimized via Genetic Algorithm

Johann Dorn

October 10, 2020

Overview **just for me**

- What is the goal
- What is the status
- What are the optimazable parameters
- What is a genetic algorithm
- What are the parameters for a GA
- Plan

What is the goal?

- ZrO_2 film via doctor blading on steel
- should be insulating (no cracks or holes)
- minimum thickness of 200 μm

What is the status?

- lower heating rate produces less cracks
- composition of starting solution

What are optimizable parameters?

- Volume:
  - Zr isopropoxide
  - AcAc
  - iPrOH
  - H2O
  - Base? organic? for pH regulation
  - Acid?
  - Surfactant?
  - high molecular co-polymer?

What are optimizable parameters?

- Volume:
  - Zr isopropoxide
  - AcAc
  - iPrOH
  - H2O
  - Base? organic? for pH regulation
  - Acid?
  - Surfactant?
  - high molecular co-polymer?
- Time:
  - Mixing Time
  - waiting before spreading
- Temperature:
  - Heating rate
  - Calcination holding time
  - Max temperature
  - Heating method oven/hot plate

What is a genetic algorithm?

- population of individuals (experiments)
- genes (experiment parameters)
- fitness (grade of satisfying the demands)
- only the fittest survive
- the individuals pair and produce offspring
- mutations

How does a GA work?

1. random initial population
2. calculate fitness
3. select pairs to become parents
4. mixing of their genomes via cross over
5. mutate the offspring genomes
6. replace old with new population
7. go to step 2

What are the parameters for GA?

- size of initial population (2-4 fold of genes)
- how is the fitness calculated?
- how are the parent pairs selected?
- crossover probability or rate
- mutation rate
- how is the population replaced?

Plan

- 6 month $\doteq$ 24 weeks
- First 2 weeks:
  - experimentally explore search space
  - choose parameters
  - choose GA parameters and write code
- 20 weeks: 10-20 generations
  create data for generations
- 2 weeks buffer

Status report: Insulating zirconia oxide layers on steel

Johann Dorn

December 1, 2020

Introduction

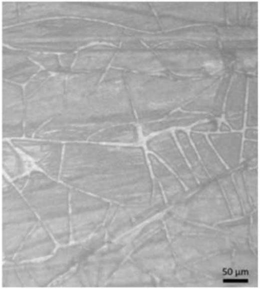
- Project: **InnovaSteel4CIGS** (AIT - Sunplugged)
- **C**opper**I**ndium**G**allium**S**elenide
- Objective:
  - Insulating coating for stainless steel
  - ZrO_2 and/or Al_2O_3
  - Scalability for industry
- application: insulation between CIGS cell and steel foil

Starting point

4th International Conference on Mechanical Engineering Research (ICMER2017) IOP Publishing
IOP Conf. Series: Materials Science and Engineering **257** (2017) 012087 doi:10.1088/1757-899X/257/1/012087

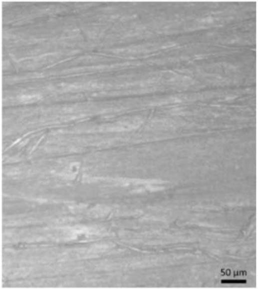
Morphology evaluation of ZrO_2 dip coating on mild steel and its corrosion performance in NaOH solution

M A Anwar[1,] T Kurniawan[1], Y P Asmara[1], W S W Harun[2], A N Oumar[3], A B D Nandyanto[4]



(a) 3 dipping

(b) 5 dipping

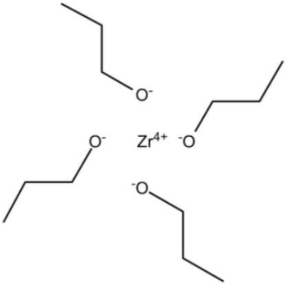


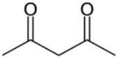
(c) 7 dipping

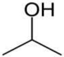
Recipe and Parameters

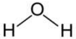
Recipe 1:

- 8ml $Zr(OPr)_4$
- 8ml AcAc
- 2ml i-PrOH
- 2.6ml H2O









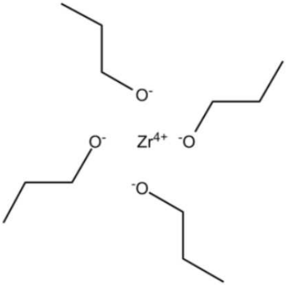
Recipe and Parameters

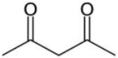
Recipe 1:

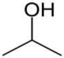
- 8ml $Zr(OPr)_4$
- 8ml AcAc
- 2ml i-PrOH
- 2.6ml H2O

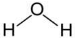
Parameters:

- Heating rate
- calcination temperature
- Mixing time
- pH regulator
- Surfactant
- High molecular polymer

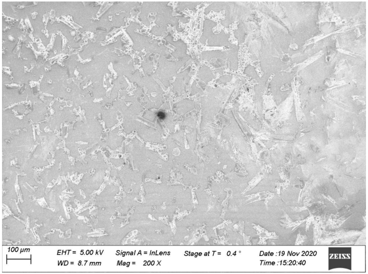




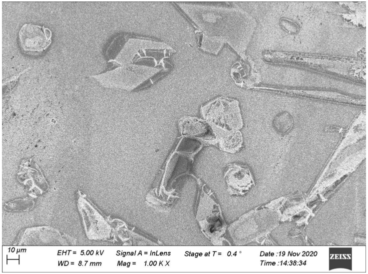




SEM results



100 µm
EHT = 5.00 kV
WD = 8.7 mm
Signal A = InLens
Mag = 200 X
Stage at T = 0.4 °
Date :19 Nov 2020
Time :15:20:40
ZEISS



10 µm
EHT = 5.00 kV
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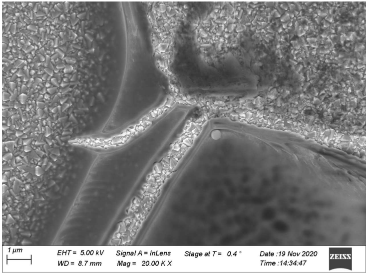
ZEISS



1 µm
EHT = 5.00 kV
WD = 8.7 mm
Signal A = InLens
Mag = 20.00 K X
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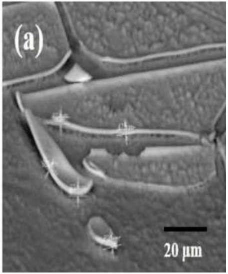
ZEISS



(a)
20 µm

Adapted recipe 2

Ceramics International 42 (2016) 16867–16871

Contents lists available at ScienceDirect

Ceramics International

journal homepage: www.elsevier.com/locate/ceramint

A new sol-gel route to prepare dense Al_2O_3 thin films

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

School of Physics and Electronic Information Engineering, Henan Polytech University, Jiaozuo 454000, China

Recipe 2:

- 9.9ml 1-BuOH
- 0.1ml $Zr(OPr)_4$
- 0.025 AcAc
- 2ml AcOH

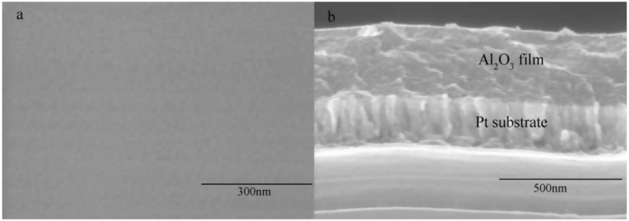
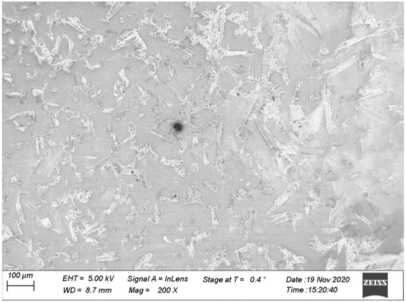
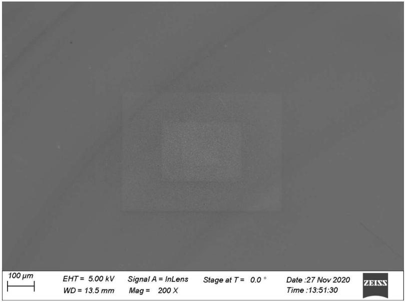


Fig. 6. FE-SEM micrograph of surface (a) and cross section (b) of an Al_2O_3 film.

SEM results

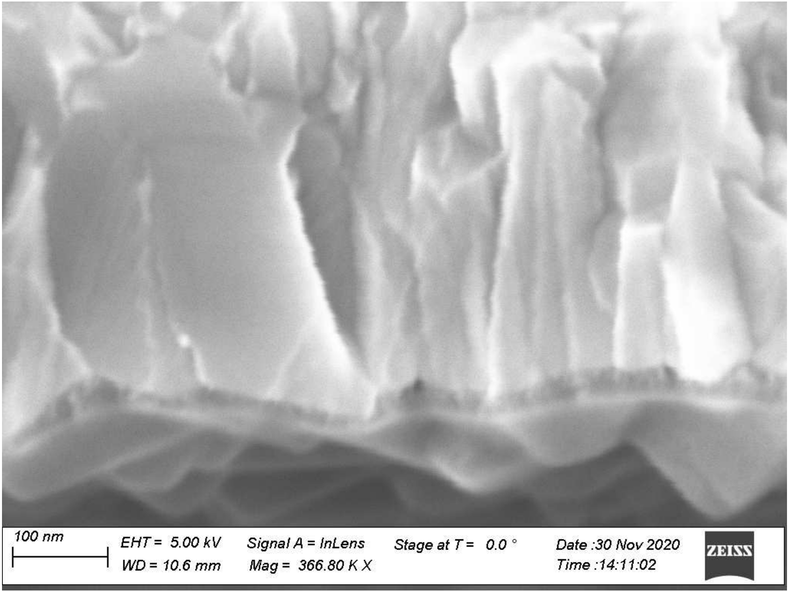


(a) Recipe 1



(b) Recipe 2

SEM cross section



Summary and Outlook

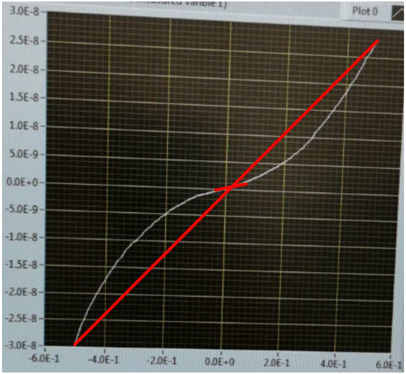
- 100nm layer
- dielectric properties: I-V, C-V
- optical spectrometry
- XRD
- Machine Learning

Sol-gel ZrO_2 film optimization

Johann Dorn

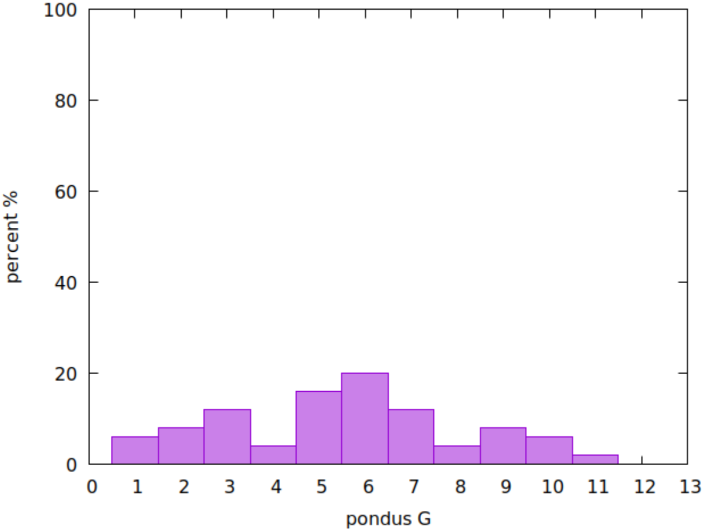
March 5, 2021

Calculation

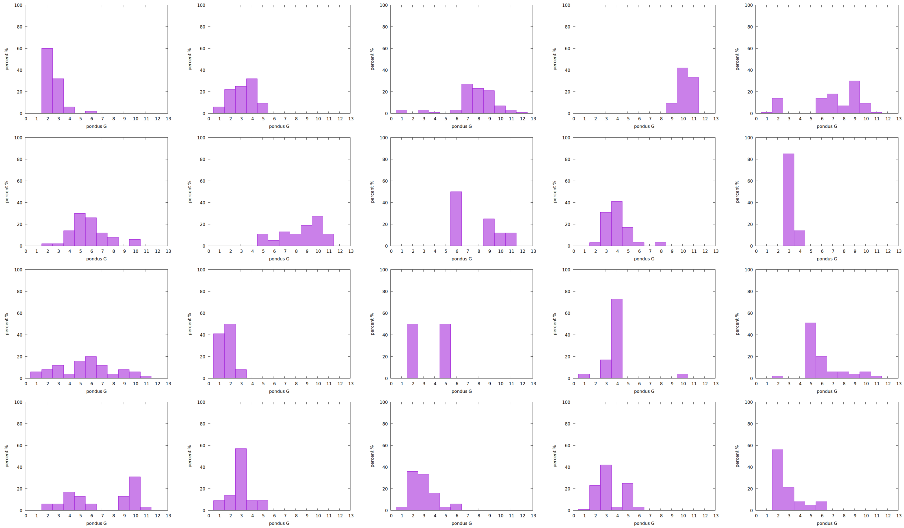


- G $= \frac{dI}{dV}$ = 4.234E-6
- G' = log(|G|) = -5.37
- pG = -log(|G|) = 5.37
  pondus,power,potential
- Q: which points best for dV
- min max overestimation ?
- average ?

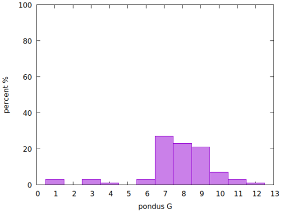
Statistics



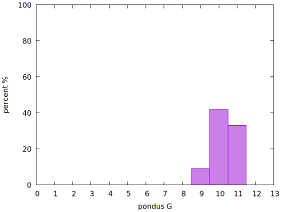
Statistics



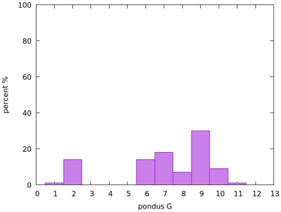
Best of



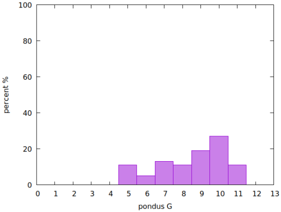
(a) 146, 10x1F HG



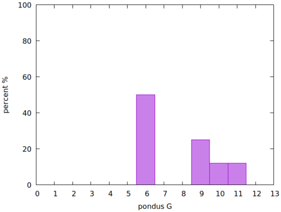
(b) 150, 5x2F HG



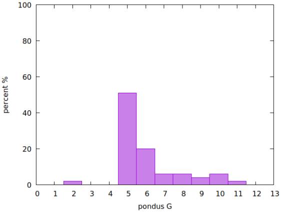
(c) 151, 2x2F HG



(d) 153, 3x4F HG



(e) 154, 3x4F HG



(f) 187, 10x1F 5mm/s

Optimazation parameters

- min (average of G)
- min (number of hole)
- min (layers)
- min (calcination temperature)?
- max (DB velocity)?
- max (heating rate)?

Optimization meta

- starting population 10 s
- extra entities/experiments per timestep $=5$ e
- 5 time steps
- $1*10+(5\text{-}1)*5 = 10+4*5 = 10+20 = 30$
- 20-30 extra samples for comparison
- approx 2-3 hours per sample

All questions

- where should be threshold be for holes?
- how to calculate derivative?
- boundaries for Tcal = [300:500] [400:500] ^oC
- layers = [6:14] [4:10]
- conc = [2:5] [1:5]
- vDoc = [10:20] mm/s
- TDOC = [40:80] ^oC
- vCal = [2:16] ^oC/min
- extra steel foil