# 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 $\mu$m

# 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 $\hat{=}$ 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