Influence of the crystallographic properties on the ionic conductivity of YSZ thin films

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Use of YSZ as ionic conductor

Stabilization of YSZ in a cubic phase:
- High ionic conductivity
- Low electrical conductivity
- High density
- Mechanical strength

YSZ as ionic conductor:
- Produces electricity directly from fuel
- Green energy
- Efficiency up to 70%
- Working temperature: 700 - 1000°C
YSZ thin film deposition using magnetron sputtering

Chamber conditions:

distance$_Y$ = 80-240 mm

current $\gamma$ = 0.2 A

distance$_{Zr}$ = 90 mm

current $\zeta$ = 0.5 A

flow$_{O_2}$ = ~2.5 sccm

$p_{Ar}$ = 0.5 Pa

Substrate = glass or Si
YSZ samples: biaxial alignment

Out-of-plane aligned

Biaxially aligned

in-plane orientation
out-of-plane orientation
grain boundary

Use of YSZ as ionic conductor
YSZ thin film deposition
Macroscopic analysis
Nanoscale analysis
Model
Impedance spectroscopy
Summary
## Macroscopic analysis

**YSZ samples** | **Y T-S distance [mm]** | **Content [at.% Y]**
--- | --- | ---
A | 240 | 11
B | 200 | 15
C | 160 | 21
D | 120 | 29
E | 80 | 38

**Use of YSZ as ionic conductor**

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**Summary**

![XRD pattern](image)

<table>
<thead>
<tr>
<th>Plane</th>
<th>Intensity (arb. units)</th>
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<td>[111]</td>
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**θ/2θ (°)**

- A
- B
- C
- D
- E
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Polar plot

Intensity (arb. units)

Composition (% at Y)

Azimuthal angle (°)

Polar angle (°)

0 10 20 30 40 50 60 70

[111] [200] [220] [311] [222] [400]
Use of YSZ as ionic conductor  
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**Pole figure**

φ: Gives the grain tilt

- **A**: Concentration of YSZ in YSZ thin film deposition.
- **B**: Polar angle (°).
- **C**: Azimuthal angle (°).
- **D**: Composition (at Y).
- **E**: Pole figure representation.
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SEM/Cross section

A

B

C

D

E

Gives the columnar tilt

Grain and columnar tilt

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![Diagram of YSZ structure with Y and Zr ions showing grain and columnar tilt.](image)

Graph showing the tilt degree versus composition (% at Y) with data points for grain tilt and columnar tilt.
Nanoscale analysis

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- YSZ FILM
- Gradient of composition
- GLASS SUBSTRATE
- 760 mm
- Zr
- Y

Gradient of composition
- 100 nm

Graph: Compositional gradient of the YSZ layer (at.%Y/mm)
Quantitative composition gradient on a single column

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Compositions at various distances from the column:

- **240 mm**
- **160 mm**
- **120 mm**
- **90 mm**

**Images**

- STEM-EDX images at different distances show varying compositions.
- ADF-STEM images illustrate the structural changes.
- Contour plots depict the composition gradient.
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$$\frac{1}{\rho} = \frac{3}{2h} \frac{(L_2 - L_1)}{L}$$

$$\frac{1}{\rho} = \frac{3}{2w_{col}} \frac{(a_y - a_{Zr})}{a}$$

Grain tilt

$$\beta = \frac{1}{2} a \sin \left[ \frac{3HD(r_Y - r_{Zr})}{2a} \frac{\partial C}{\partial x} \right]$$
Macroscopic and nano scale fit in the model

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Grain tilt (°) vs. Composition (at.% Y)

- Grain tilt
- YSZ layer
- Column

www.draft.ugent.be
First results with impedance spectroscopy

- Gold electrodes
- YSZ layer
- Silica layer
- Silicon wafer
- Ceramics and Platinum shielding
- Heater

**Summary**

First results with impedance spectroscopy

YSZ sample: 0.795 ± 0.01 μm / 10 at.%Y

Across-plane electrodes

In-plane electrodes

Summary
Summary

The tilt on the columnar grow is resultant of several deformed lattices on top of each other.

Via EDX-STEM and EDX-SEM we can quantitatively determine the equivalent compositional gradient on a column and on a YSZ film.

The used model allows the prediction of the grain tilt on YSZ thin films on a nanometer and macroscopic scale.

The similarity between YSZ polycrystalline and YSZ film is a strong indication that the conductivity of the film is essentially ionic.
Impedance spectroscopy:

DRAFT – colleagues