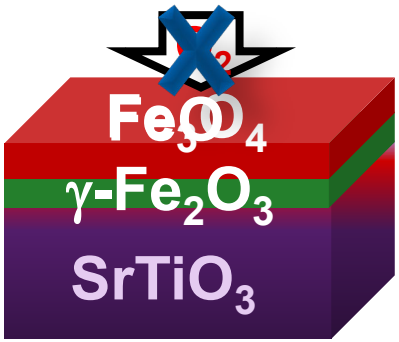
PHD DAYS PRESENTATION

Influence of substrate on the redox behavior of Fe_3O_4/Oxide substrate heterostructures

JCNS-2 FORSCHUNGSZENTRUM JÜLICH
Heinrich Heine University Düsseldorf

15.02.2022 I *Yifan Xu*

Thin film phase diagram



2nm
2nm

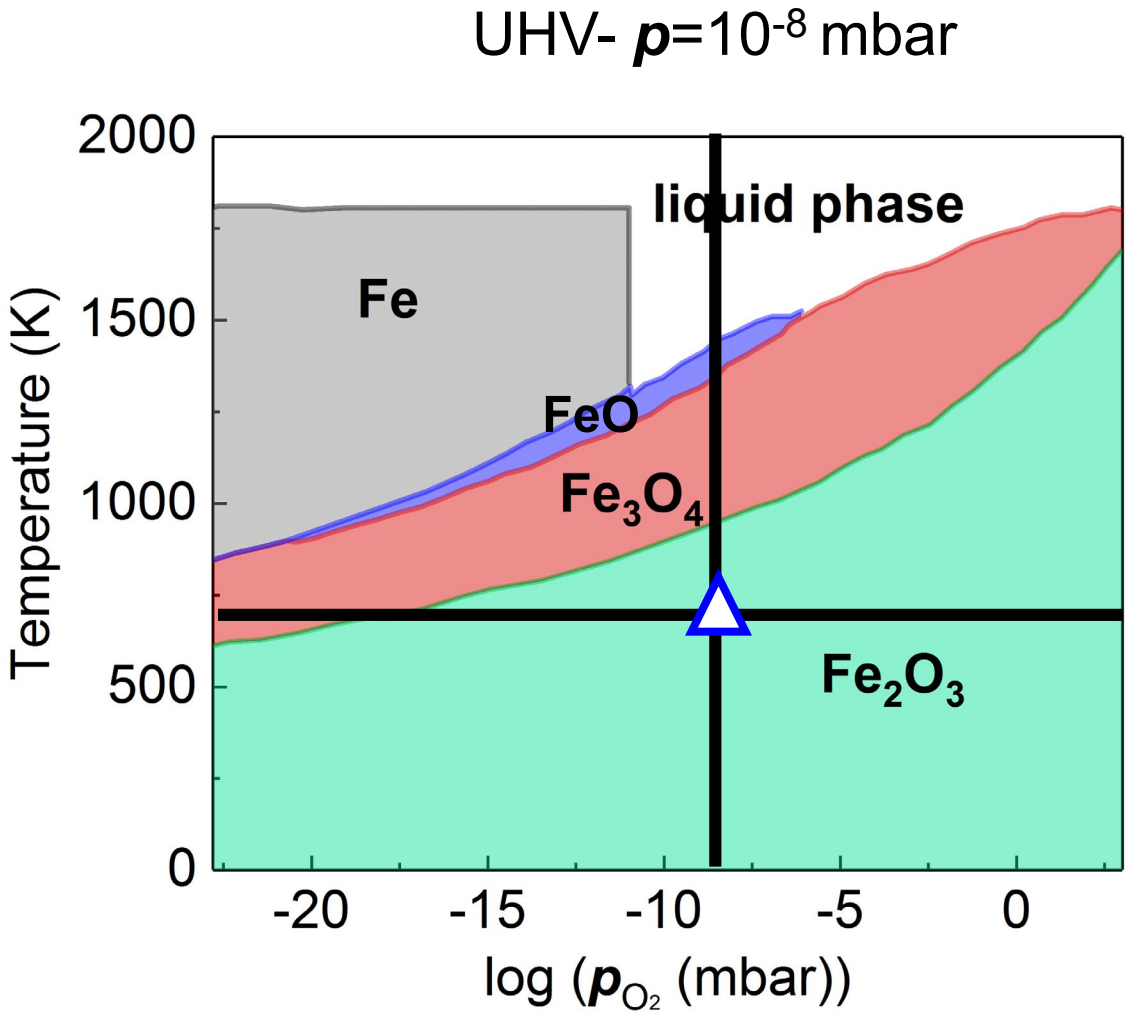
T_{anneal}=400 °C

Three relevant interfaces:

~~(1) Atmosphere/Fe_xO_y~~

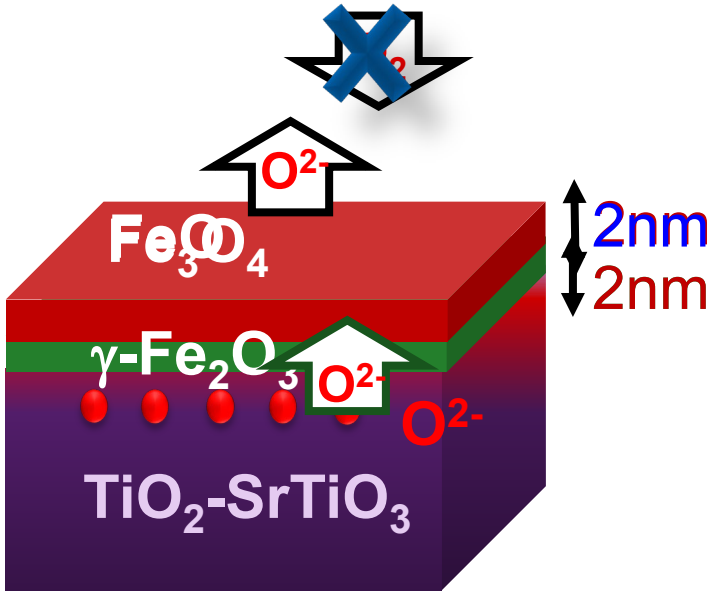
(2) Fe_xO_y/Fe_xO_y

(3) Fe_xO_y/Oxide substrates

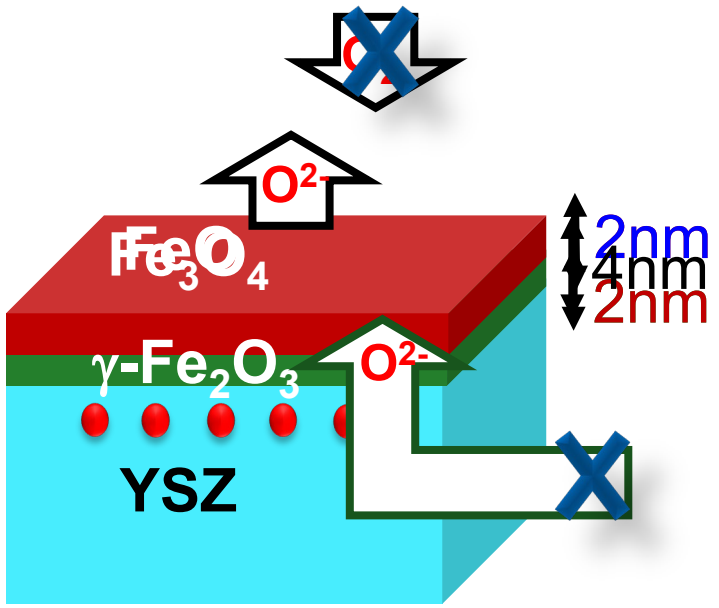


Hamed, M. H., Mueller, D. N., & Müller, M. (2020). Journal of Materials Chemistry C, 8(4), 1335-1343.

Redox Reaction Influenced by Oxide Substrates



- Reducible



- Hardly reduced
- Good oxygen conductor

Hamed, M. H., Mueller, D. N., & Müller, M. (2020). Journal of Materials Chemistry C, 8(4), 1335-1343.

QUESTIONS

Three relevant interfaces:

~~(1) Atmosphere/Fe_xO_y~~

(2) Fe_xO_y/Fe_xO_y

(3) Fe_xO_y/Oxide substrates

→ Depth profile?
XRR, PNR

Structure, crystallinity?
→XRD

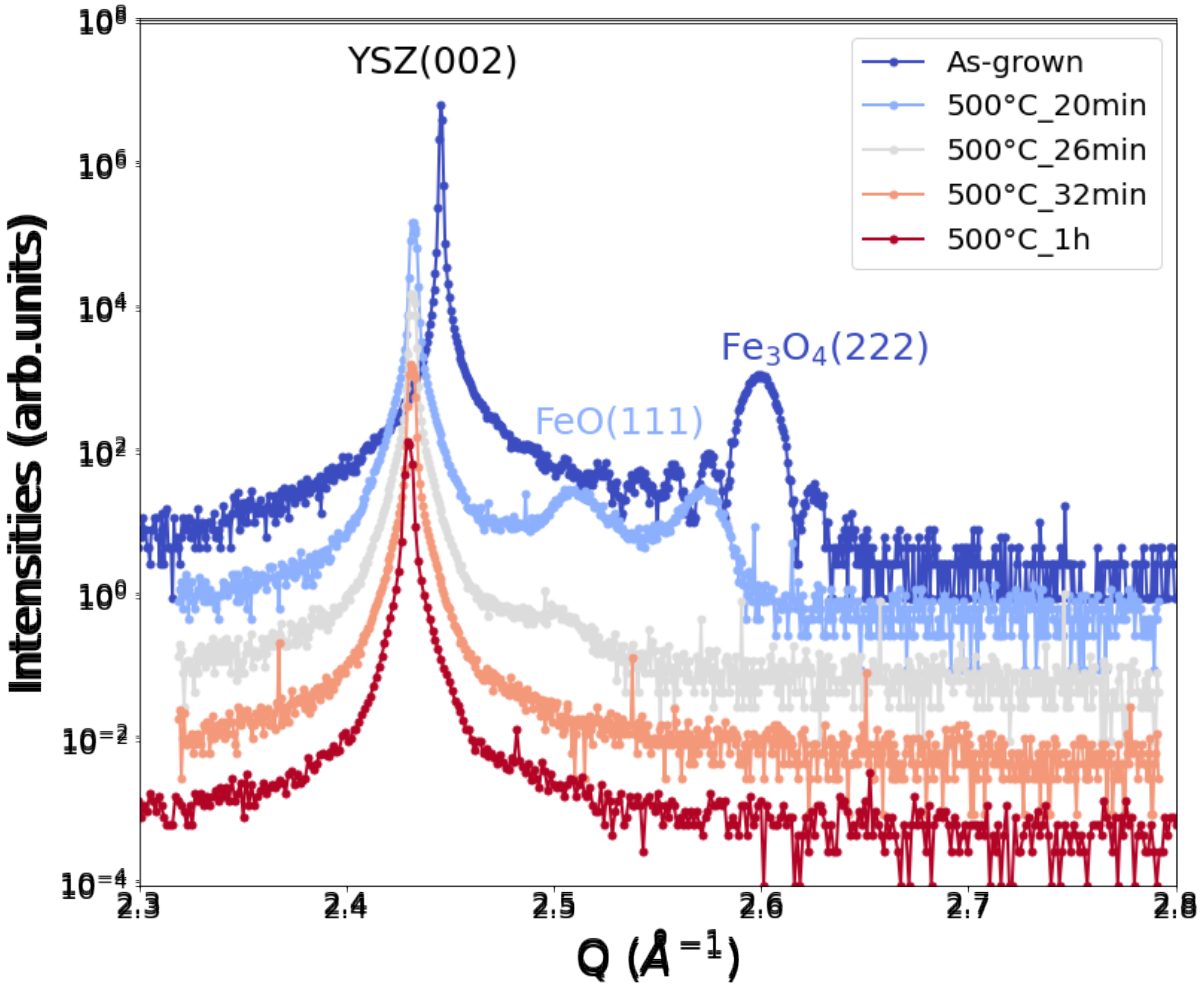
Magnetic?
→PNR

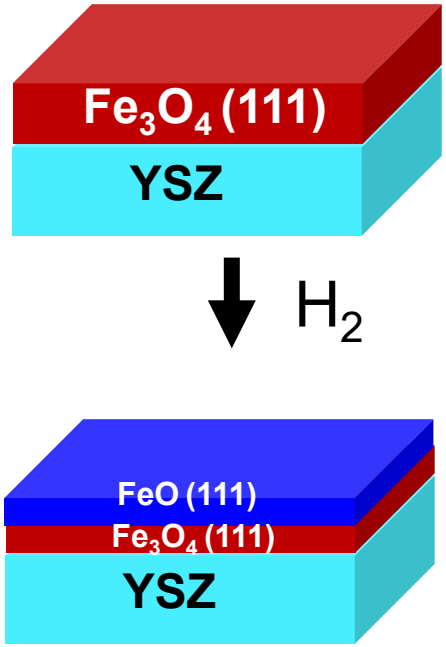
Fe_3O_4 (30nm)/ **YSZ** vs.
Fe_3O_4 (30nm)/ **TiO_2-STO**
→ **Redox behavior while annealing**

XRD

YSZ / TiO_2-STO

Base pressure: $1e^{-2}$mbar
4% H_2 with Ar

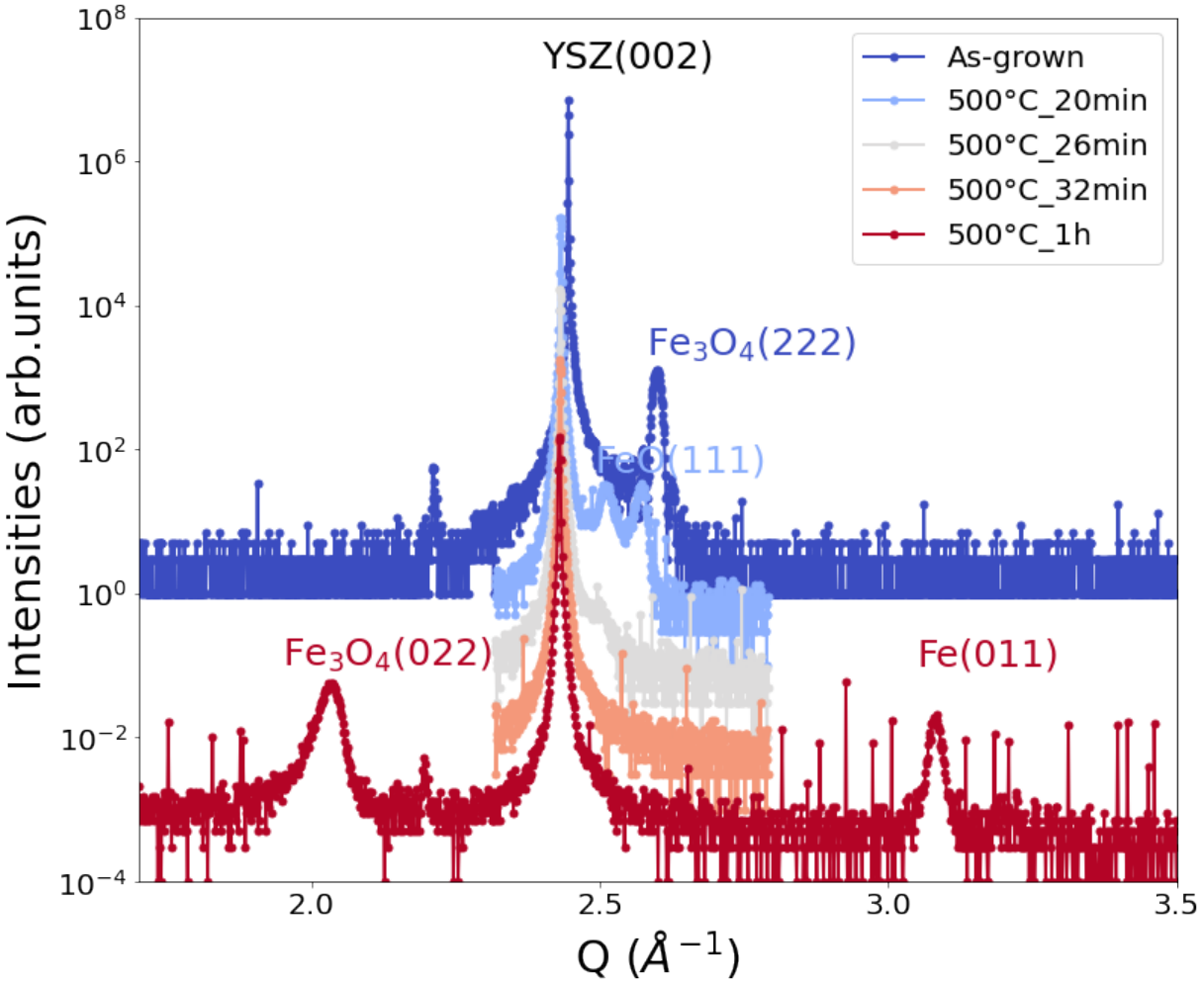


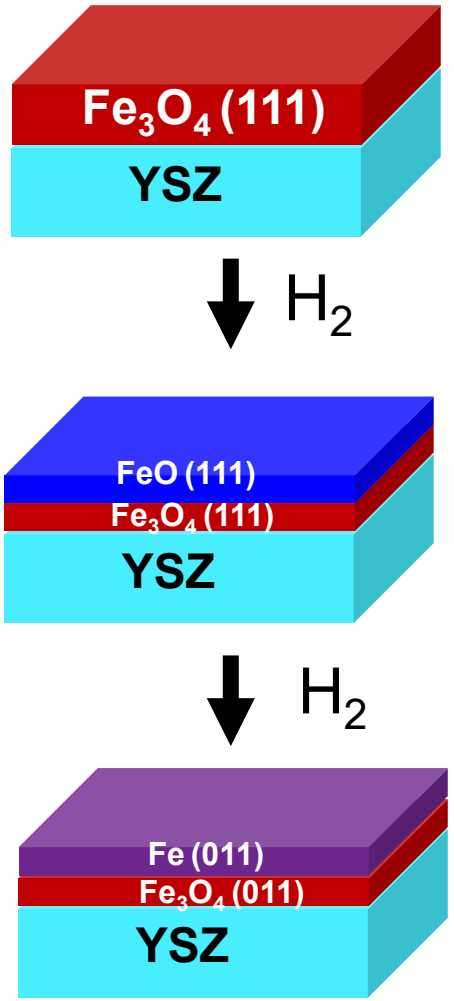


Experiment assisted by Felix Gunkel (PGI-7)

XRD

YSZ / TiO_2-STO

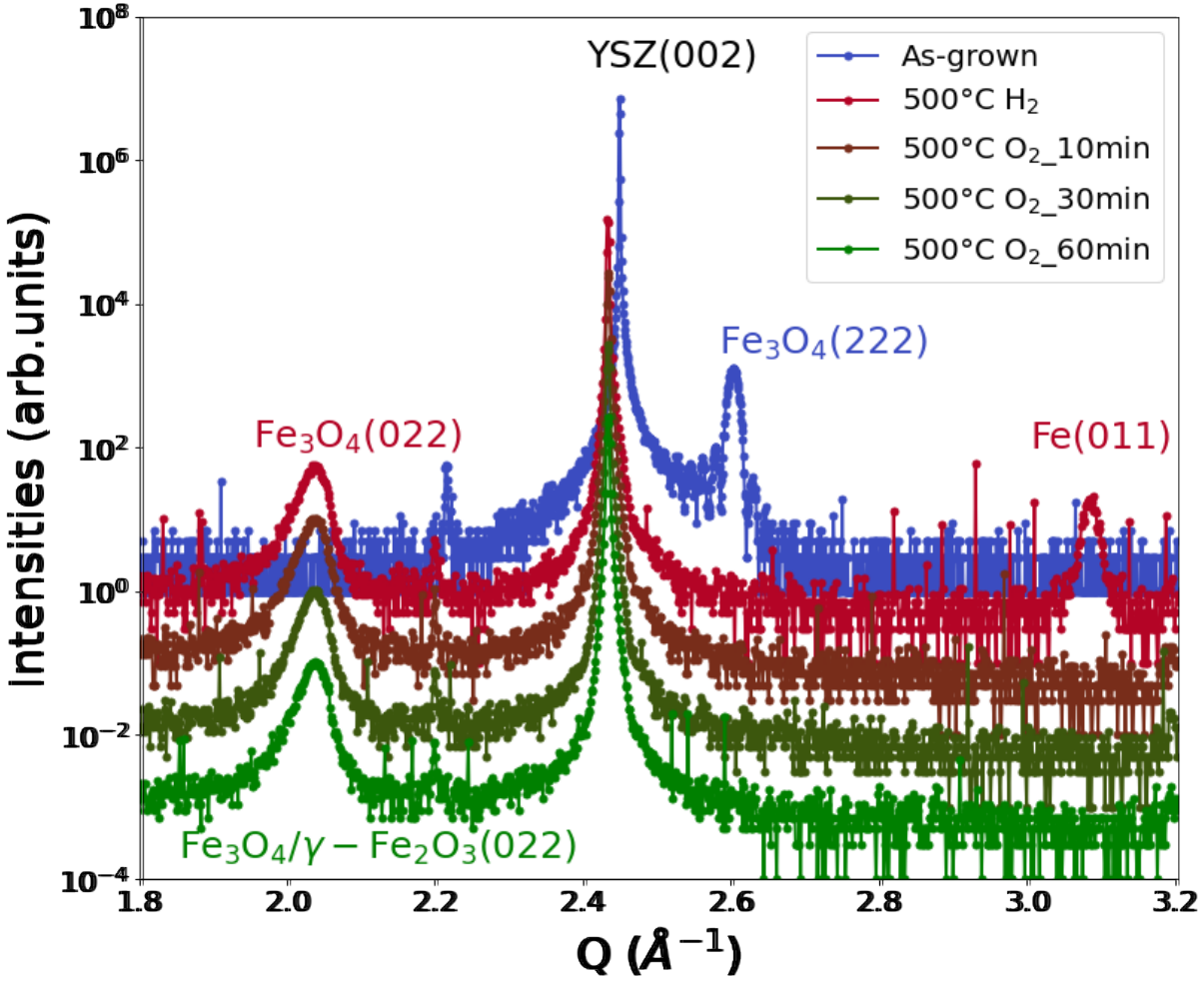


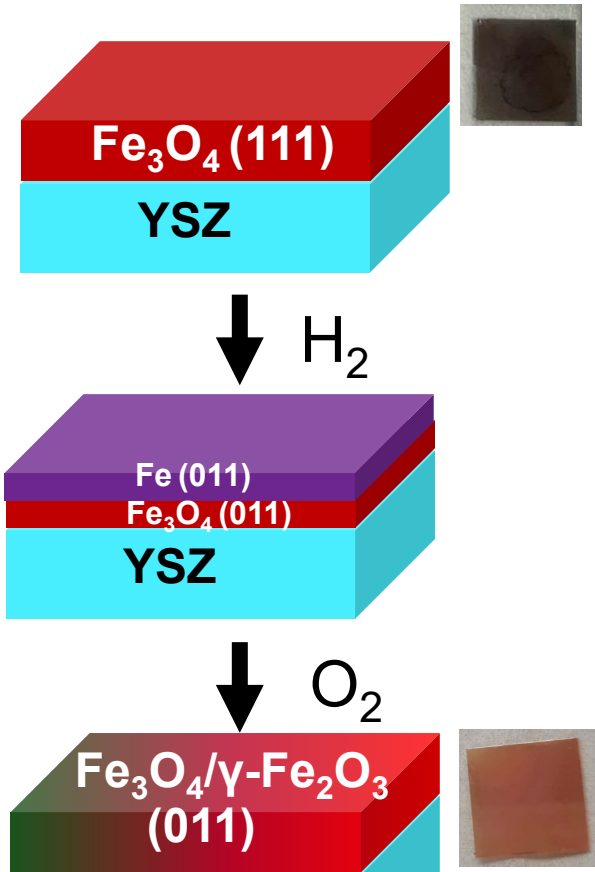


Experiment assisted by Felix Gunkel (PGI-7)

XRD

YSZ / TiO_2-STO



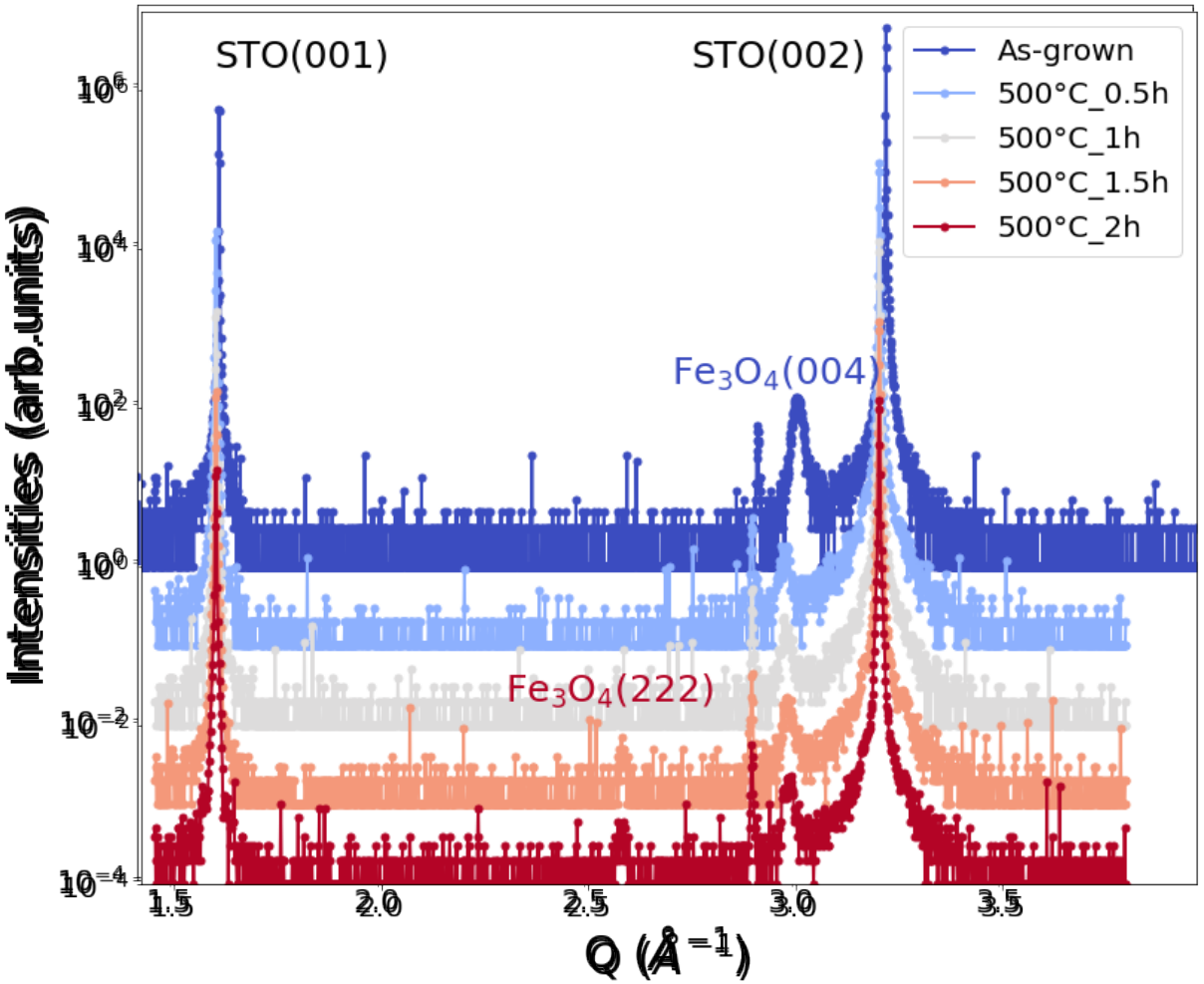


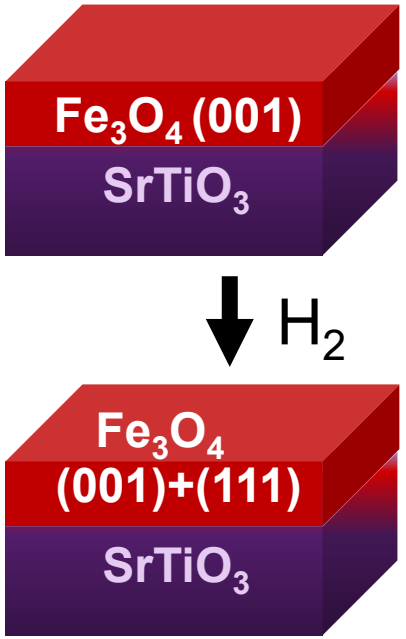
JÜLICH Forschungszentrum

Experiment assisted by Felix Gunkel (PGI-7)

XRD

YSZ / TiO_2-STO



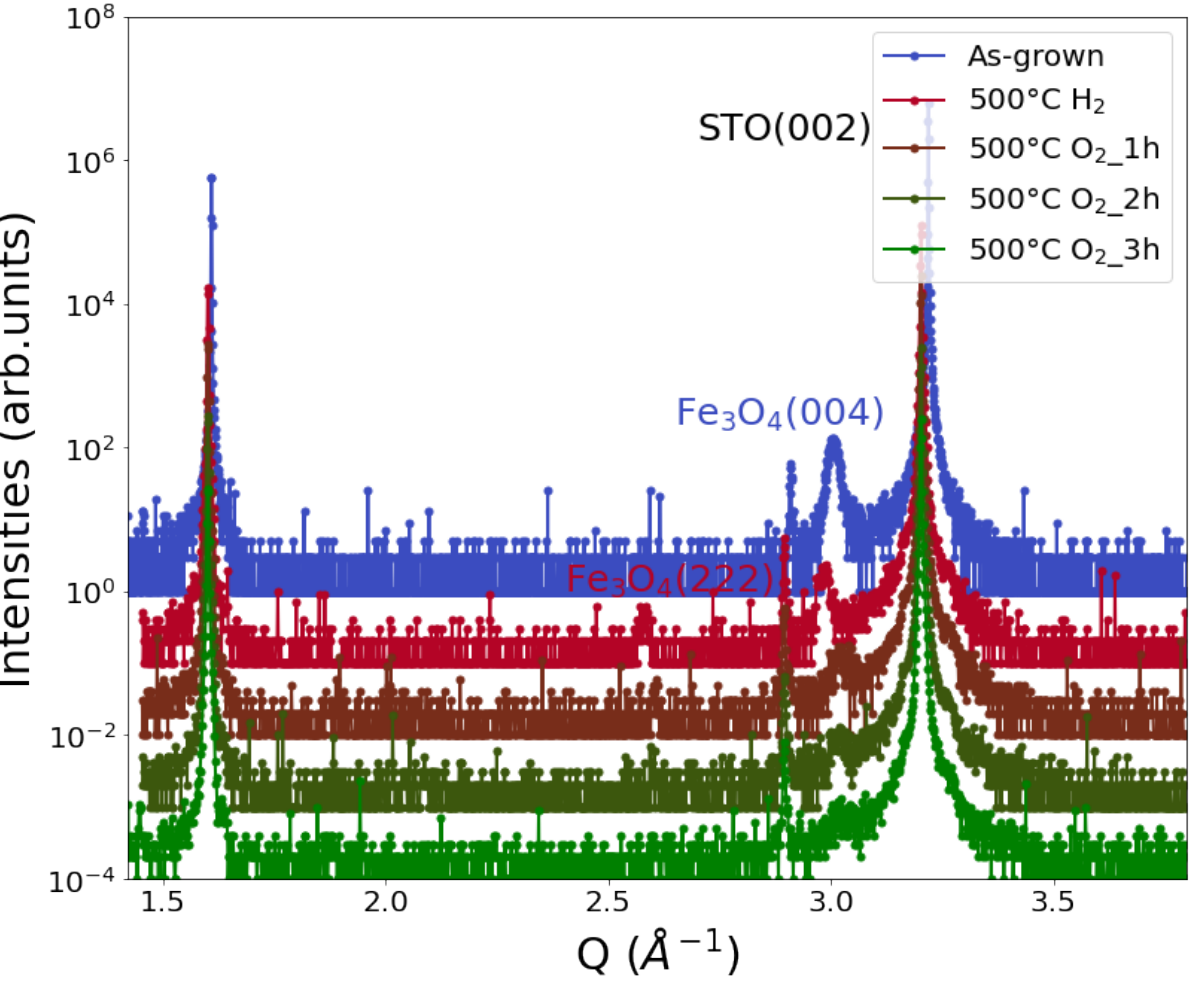


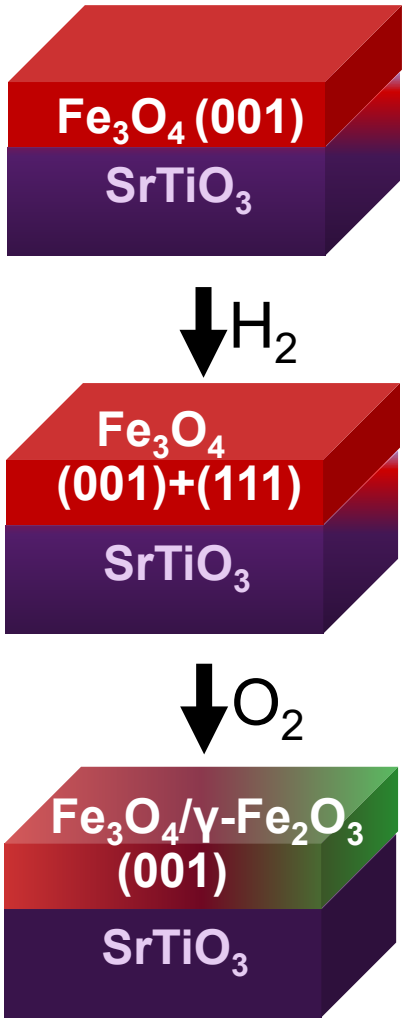
Experiment assisted by Felix Gunkel (PGI-7)

p ~1e^{-20}mbar

XRD

YSZ / TiO_2-STO



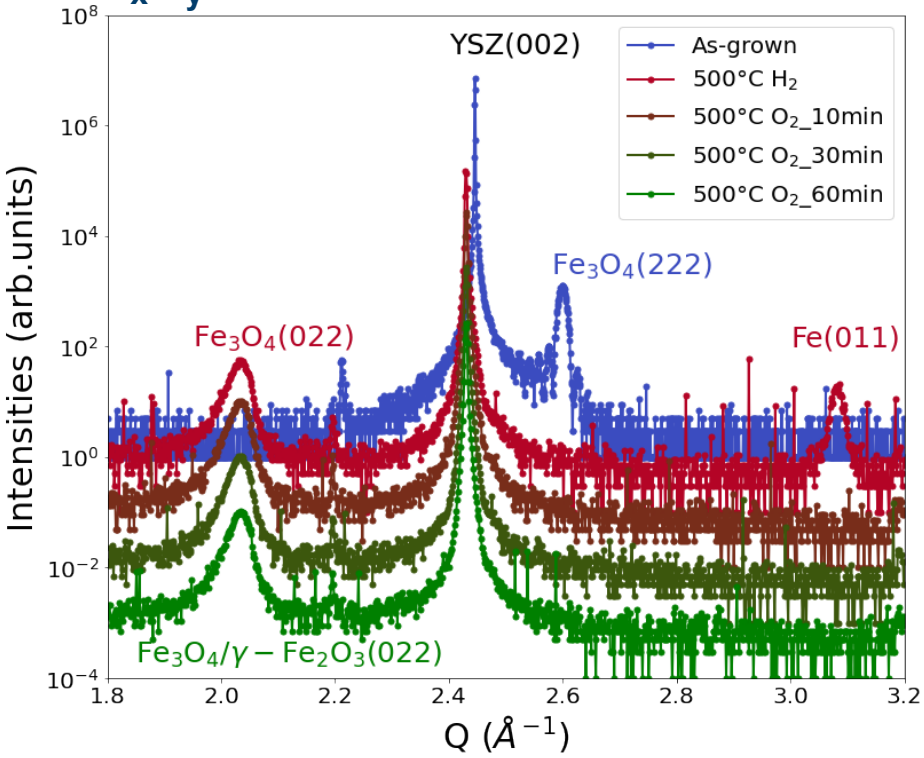


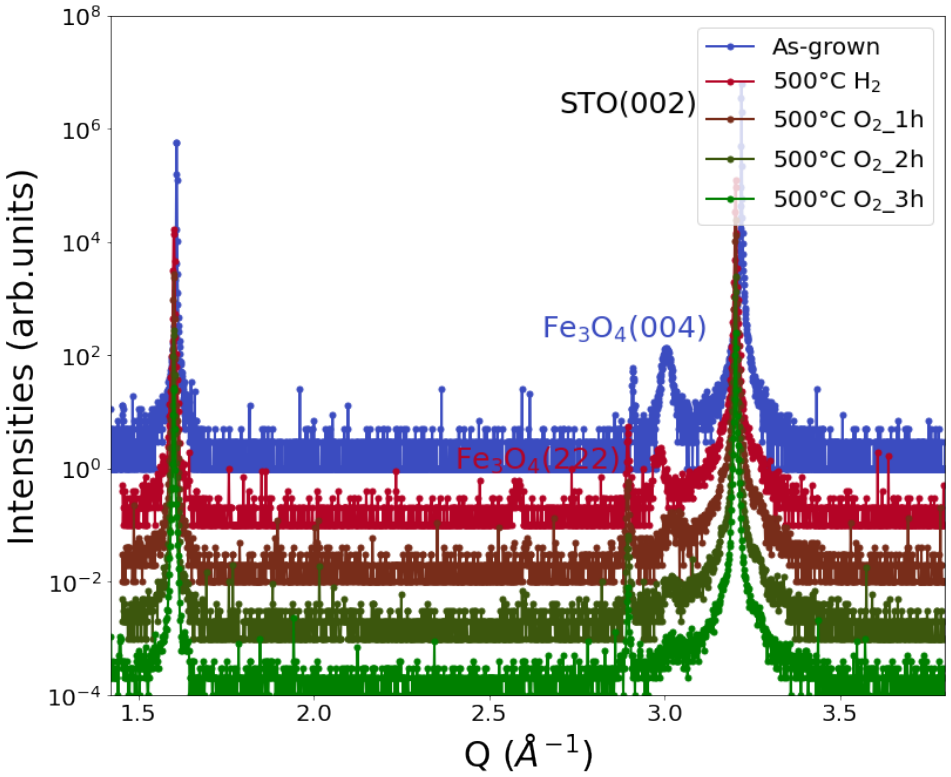
Experiment assisted by Felix Gunkel (PGI-7)

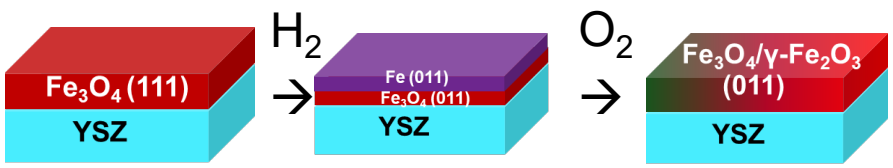
QUESTIONS

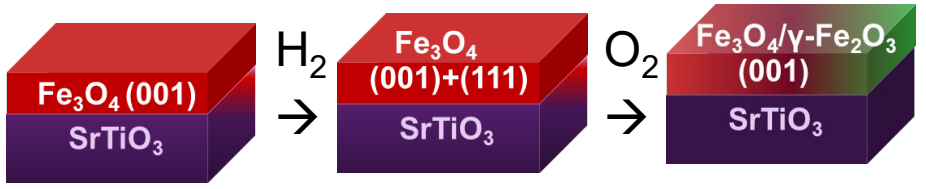
Structure, crystallinity?
→ XRD

Fe_xO_y/Oxide substrates









Experiment assisted by Felix Gunkel (PGI-7)

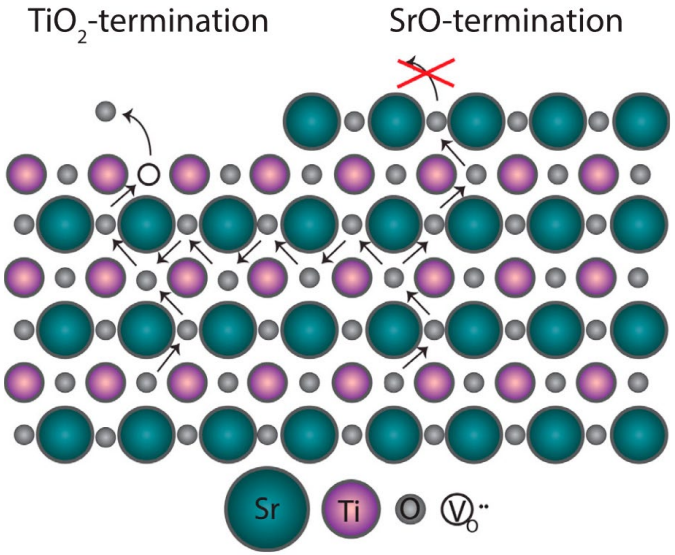
WHAT'S MORE

YSZ/ STO

1. Crystallinity:
   - Fe_3O_4 (001) / STO (001)
   - Fe_3O_4 (111) / YSZ (001)

2. Lattice mismatch:
   - ➢ -7.5 %
   - ➢ 6 %

→ Different termination of STO



$\Delta G_{Fe_3O_4}$ = -1164 kJ/mol

ΔG_{SrTiO_3} = -1500 kJ/mol

$\Delta G_{TiO_2-SrTiO_3}$ = -900~1039 kJ/mol

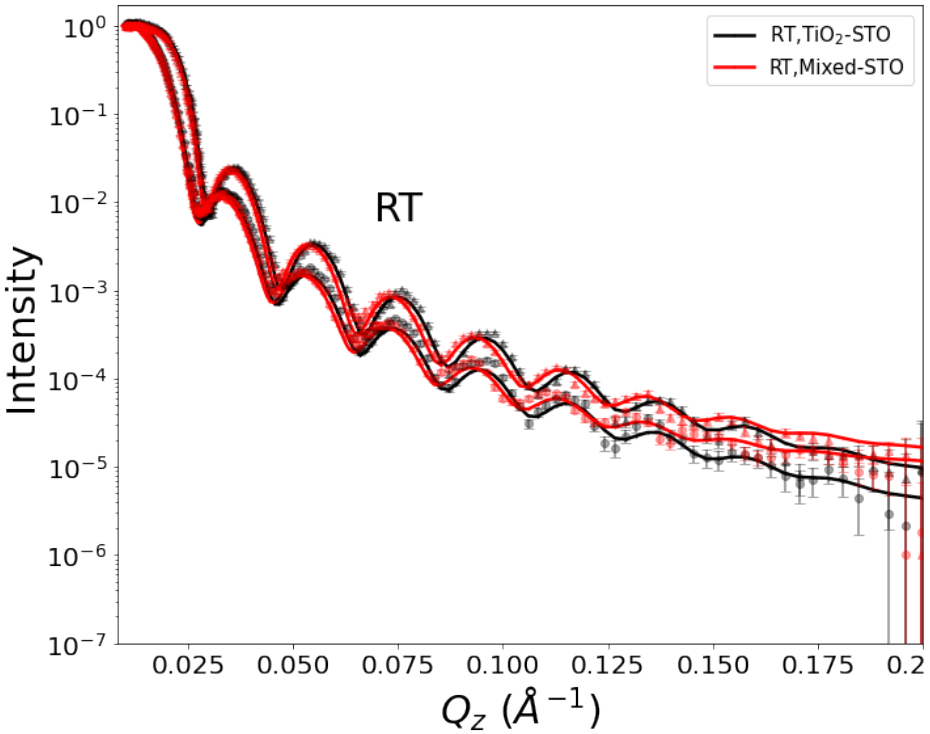
reduce

NIST-JANAF thermochemical tables (1998)
The European Physical Journal B **72**, 53 (2009)

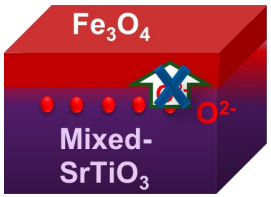
Felix V. E. Hensling, Materials Research Letters, 8:1, 31-40

PNR

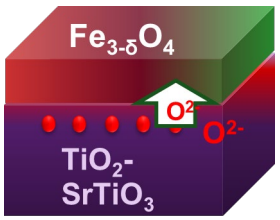
TiO_2- / Mixed- STO



- **Mixed→**



- **TiO_2- →**



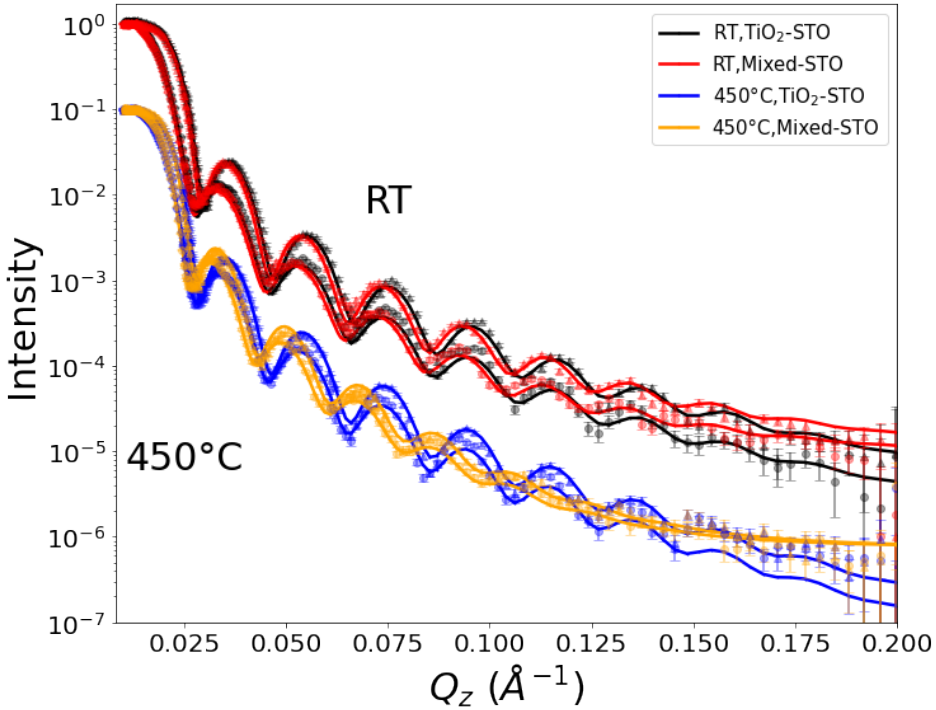
Fit by GenX with single layer model Fe_3O_4/STO

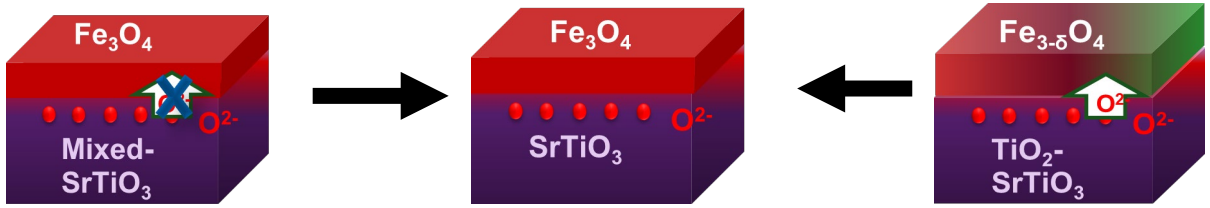
Base pressure: 10^{-6}mbar

PNR

TiO_2- / Mixed- STO

Base pressure: 10^{-6}mbar



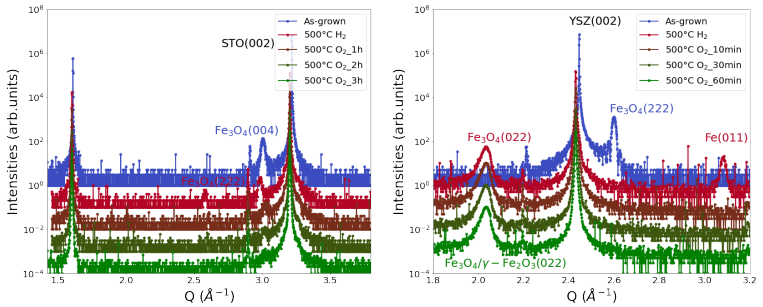


Fit by GenX with single layer model Fe_3O_4/STO

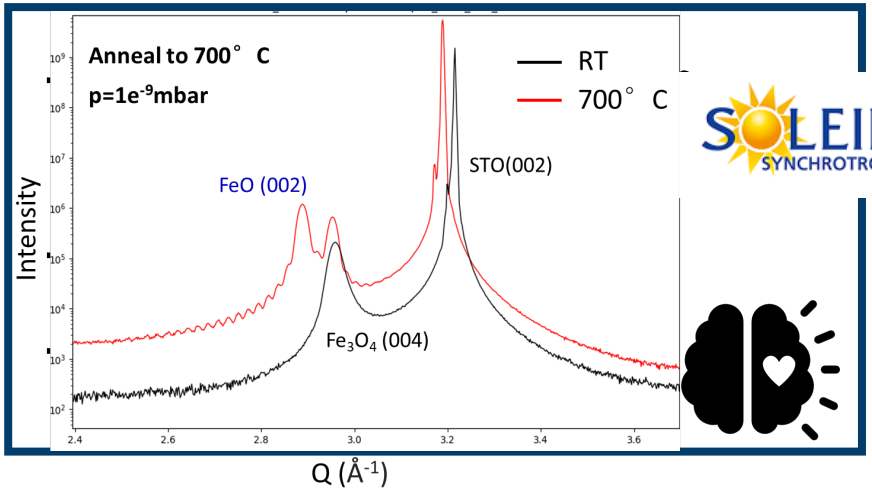
SUMMARY AND OUTLOOK

1. Fe_3O_4 (30nm)/ **YSZ** vs. Fe_3O_4 (30nm)/ **TiO_2-STO**

   - Redox reaction influenced by substrate!!
   - Preferred orientation while annealing



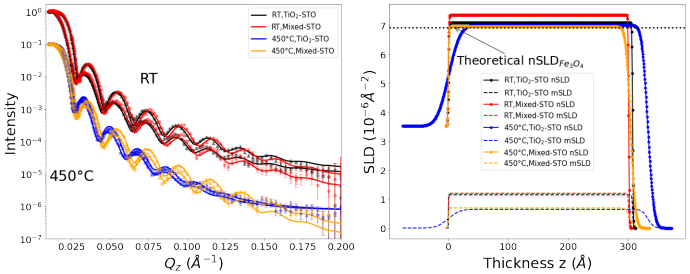
- Bad data quality for Fe_3O_4/ STO
- In-plane?
- Magnetic?



SUMMARY AND OUTLOOK

2. Fe_3O_4 (30nm)/ **TiO_2-**STO vs. Fe_3O_4 (30nm)/ **Mixed-**STO

- Difference in nSLD
- Roughness at interface ↑



- Single layer as fitting model?
- Bad vacuum of 1x10^{-6}mbar
- Un-controlled mix-termination?

→TEM and XRD

→Better vacuum

→SrO- by depositing single layer of SrO in MBE

THANK YOU

Thank you for your listening

Thanks a lot to Thomas Brückel, Regina Dittmann, Karen Friese, Mai Hussein Hamed, Connie Bednarski-Meinke, Asmaa Qdemat , Oleg Petracic, Emmanuel Kentzinger, Steffen Tober, Chenyang Yin, Suqin He, Maximilian Enneking, Ulrich Rücker, Felix Gunkel , Frank Gossen