

Theion, a high-energy lithium-sulfur technology

Our cathode chemistry

9th Workshop Lithium-Sulfur Batteries

28.11.2022

Andréa Martin

Global presence of Li-S companies



More than 25 companies developing Li-S technology

A new way how to design sulfur cathode

**Hierarchical Monolithic
Sulfur Cathode
„Sulfur Wafer“**

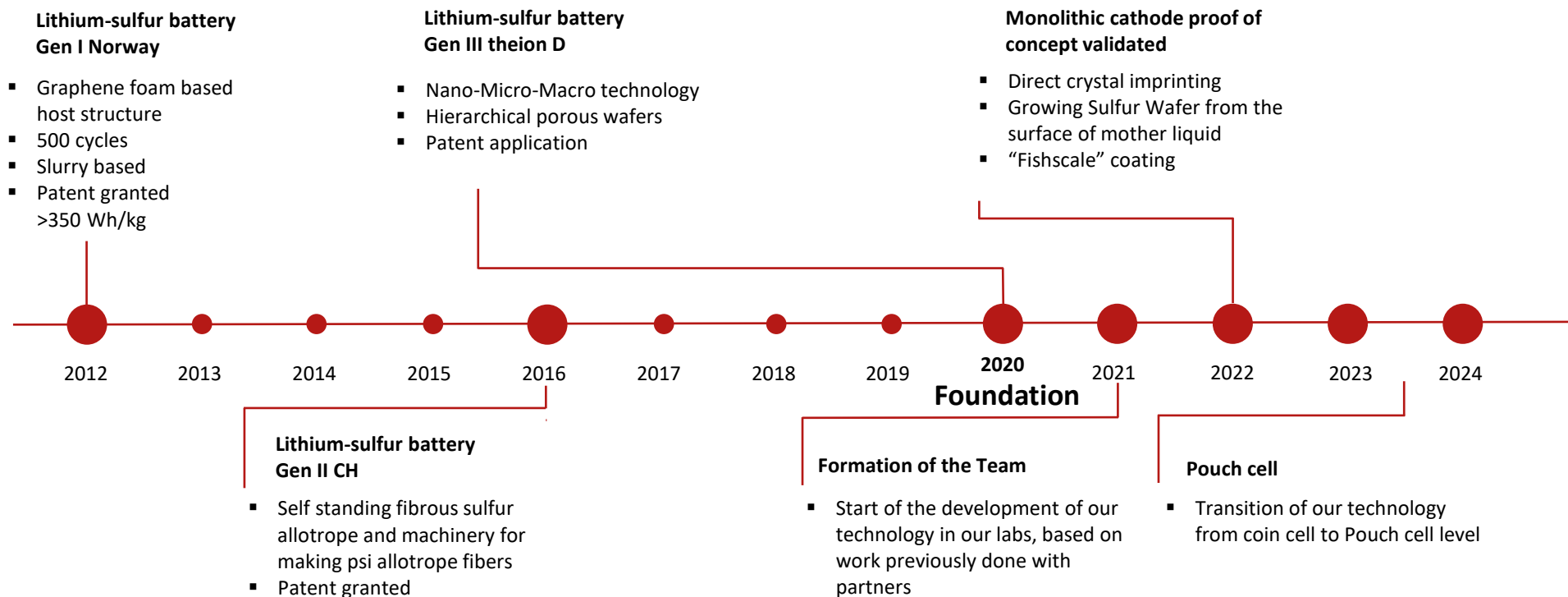
„Fishscale“ coating

**Control of the Sulfur
Chemical Structuration**

**Buffering the Volume
Expansion**

History of the company

10 years research work by CSO Marek Slavik
in Lithium-Sulfur batteries



The team

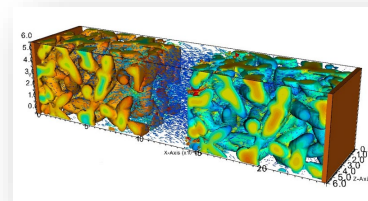
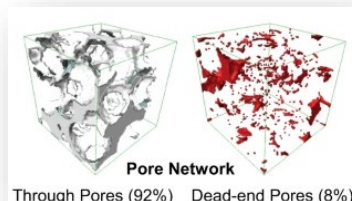


18 persons 10 nationalities

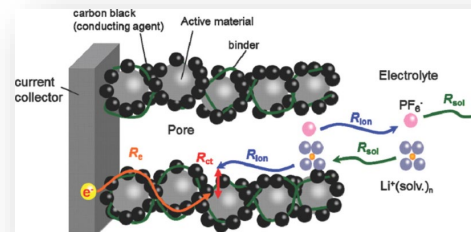
Monolithic Sulfur Cathode „Sulfur Wafer“

Slurry-based electrodes

- Random organization of the porosity
 - „clogged“ porosity where the electrolyte does not have access
 - Size of the pores not controlled: unefficient electrolyte filling ($E/S > 3\text{ml/g(S)}$)



- Random organization of percolation network
 - Tortuous diffusion of the electrons through the electrode
 - „Jumps“ of the electrons from one particles to another



Monolithic Sulfur Cathode „Sulfur Wafer“

Our strategy

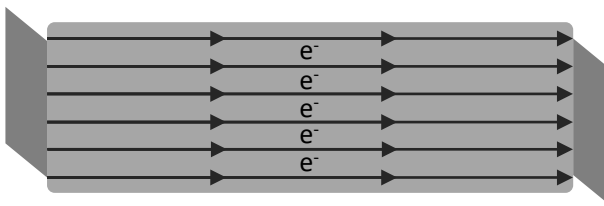
- In contrast to the state of art Sulfur cathode technology, we do not build up host structure to accomodate Sulfur, but a Sulfur matrix that we modify by different mean.



- The porosity of this Sulfur matrix can be tuned with our fabrication method



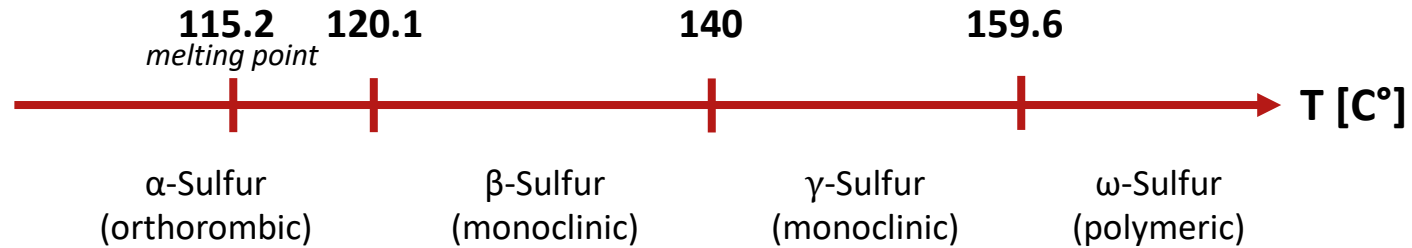
- A straightforward artificial percolation network is built up within the whole electrode



Monolithic Sulfur Cathode „Sulfur Wafer“

≡ theion

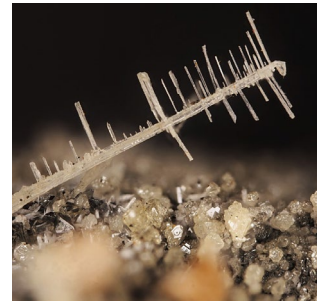
Different phases of recrystallination of Sulfur allotropes (pure sulfur at 1 atm)



α -Sulfur (orthorhombic)
3D



β -Sulfur (monoclinic)
2D



γ -Sulfur (monoclinic)
1D



ω -Sulfur (polymeric)

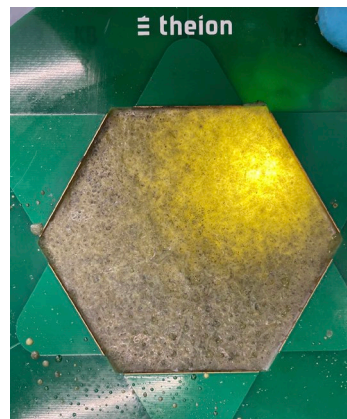
Monolithic Sulfur Cathode „Sulfur Wafer“

Made by Nature



Cristal twinning - Hyperbranching of monoclinic Sulfur

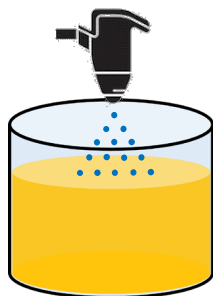
Made by Theion



Macrometric picture of a hexagonal „Sulfur Wafer“



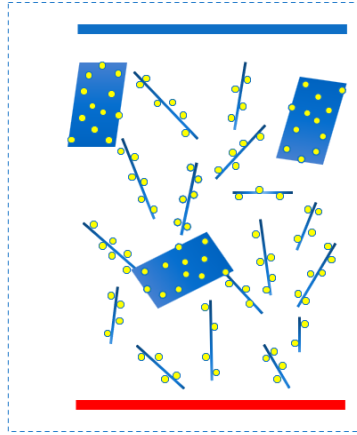
Micrometric picture of a hexagonal „Sulfur Wafer“



Through a **DCi** (**D**irect **C**ystal **i**mprinting) supported by inkjet printing and electric manipulation of conductive objects

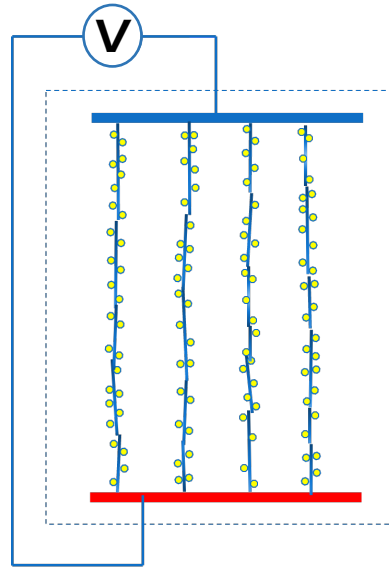
Monolithic Sulfur Cathode „Sulfur Wafer“

DCi process



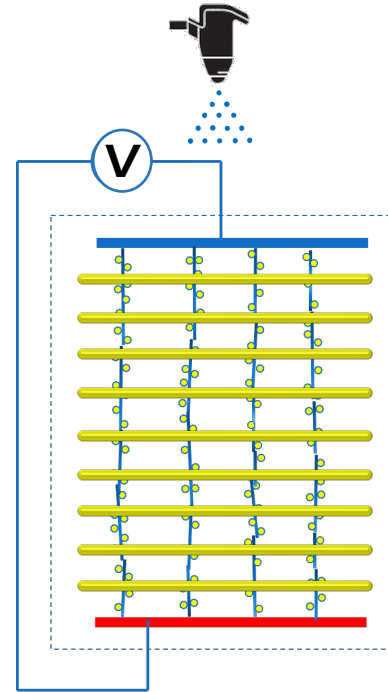
Step 1

Deposition of the conductive object decorated with nucleation points



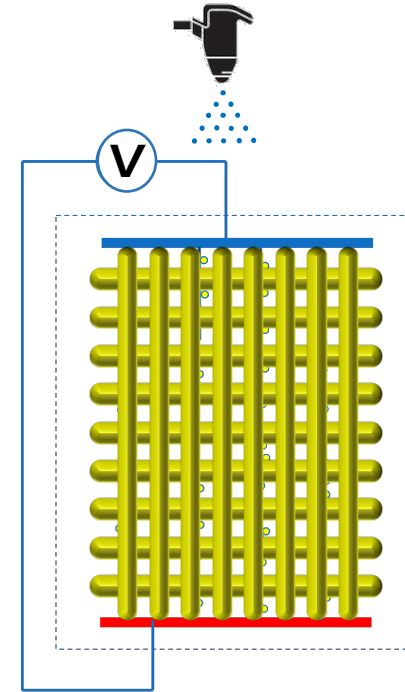
Step 2

Alignment of the conductive object under electric field



Step 3

Inkjet printing cooling and crystallization of the sulfur onto the nucleation points



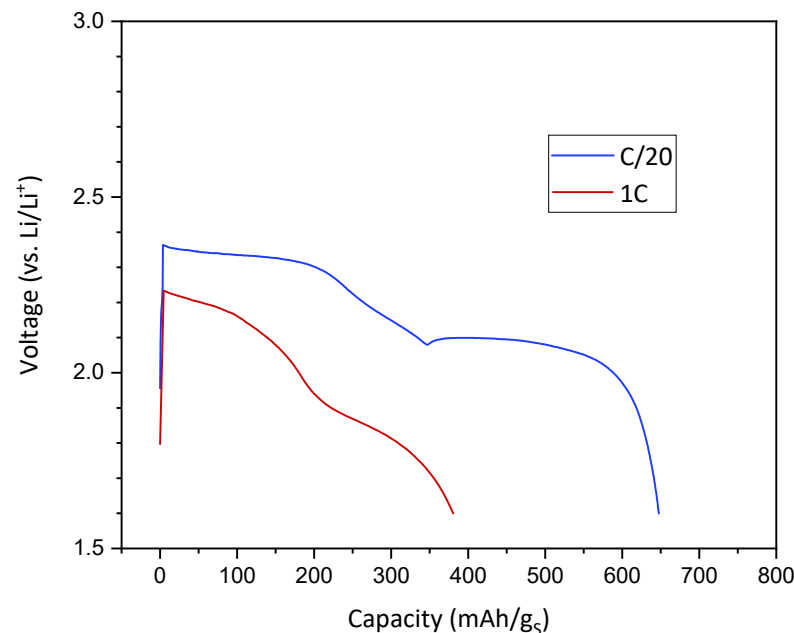
Step 4

Hyperbranching of the structure and formation of a monolith

Monolithic Sulfur Cathode „Sulfur Wafer“

With this method

- Control on the porosity of the Sulfur monolith
Possibility of obtain open porosity down to 20% → E/S
< 3ml/g(S)
- Straightforward „artificial“ percolation network
→ minimum amount of conductive additive needed



Sulfur content: **98%** ; Mass loading: **>10 mg(S)/cm² @C/20 & 1C** ; E/S = 5ml/g(S)
Coin cell level Aprotic organic based electrolyte

„Fishscale“ coating

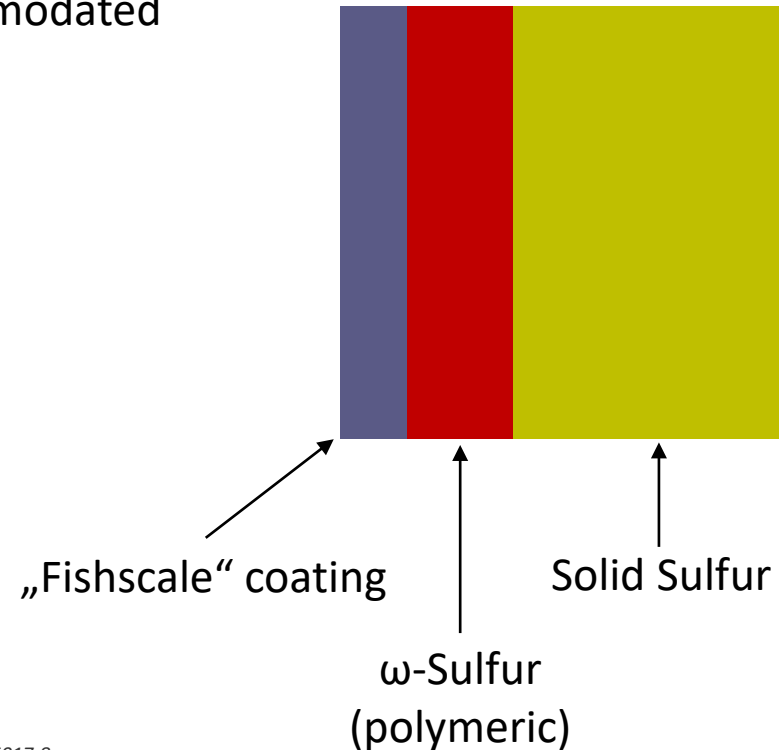
With this method

- Not host structure where Sulfur is accommodated

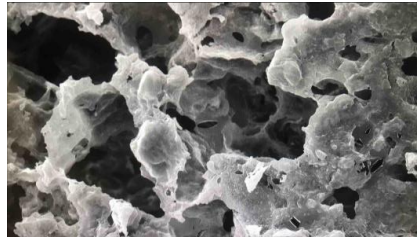
 **Lithium-Polysulfide Shuttle**

- Our solution: „Fishscale“ Coating

A conductive coating that prevents the Li-polysulfide shuttle/dissolution and is chemically bonded to Sulfur

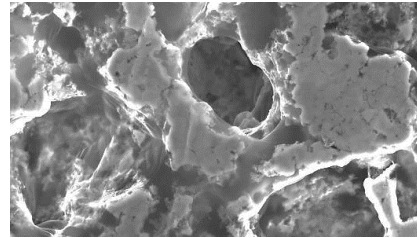
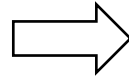


„Fishscale“ coating



Scanning Electronic Microscopy Image
of Sulfur matrix

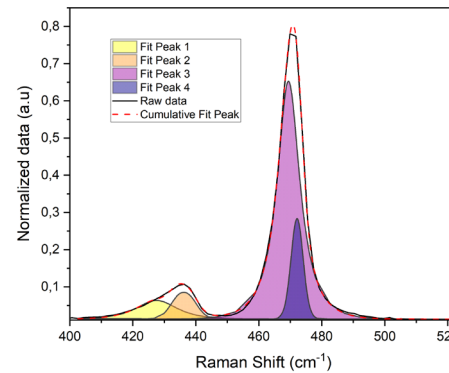
Coating



Scanning Electronic Microscopy Image
of coated Sulfur matrix

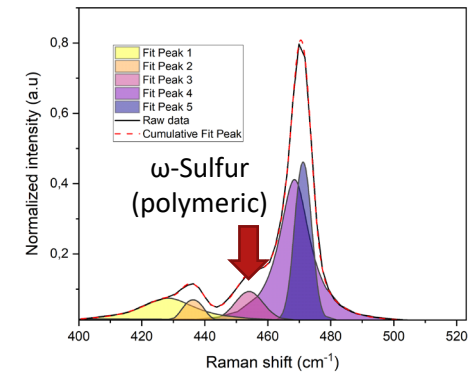
Stabilization of ω -Sulfur
(polymeric) through cross-linking
reaction between the „Fishscale“
coating and Sulfur (but also
enhancement of the electronic
properties).

Before special treatment, the
coating is only physically
attached to the Sulfur Matrix.



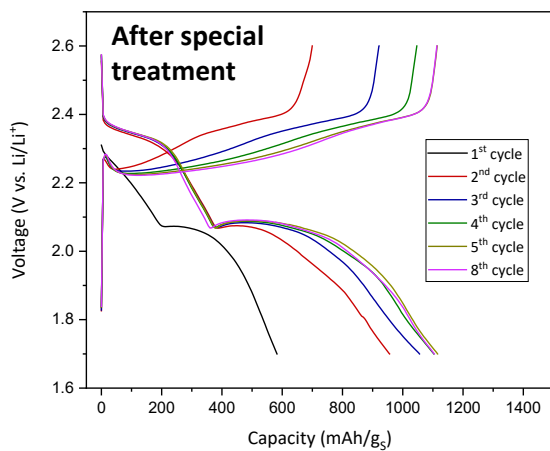
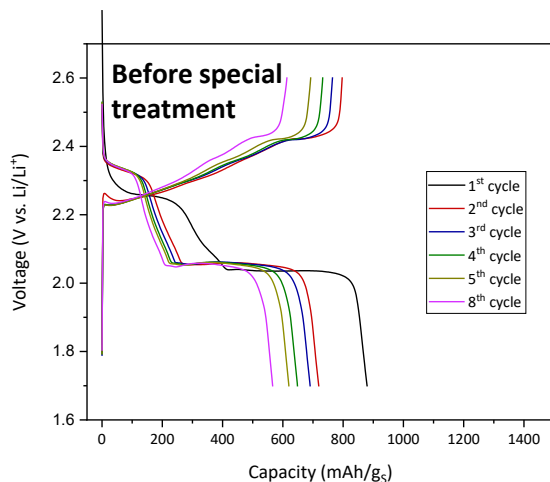
Raman Spectra of coated Sulfur Matrix before special
treatment

Special
treatment



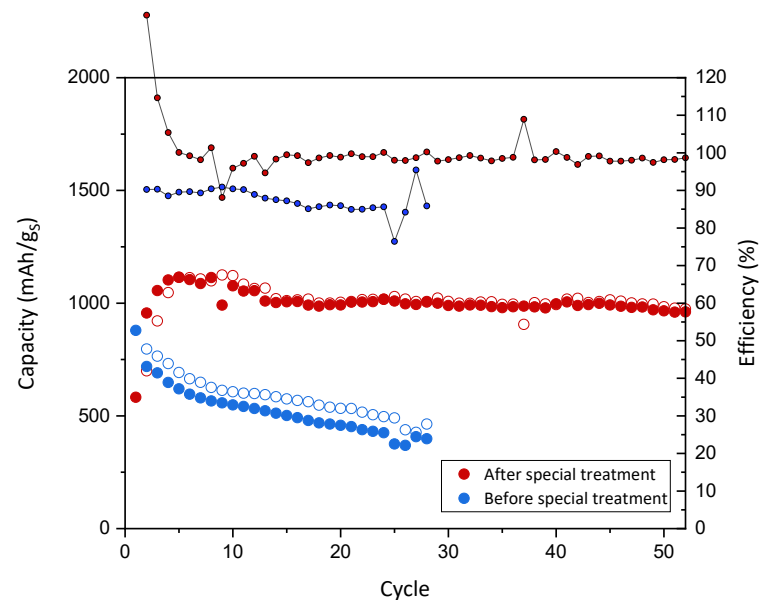
Raman Spectra of coated Sulfur Matrix after special
treatment

„Fishscale“ coating



After special treatment

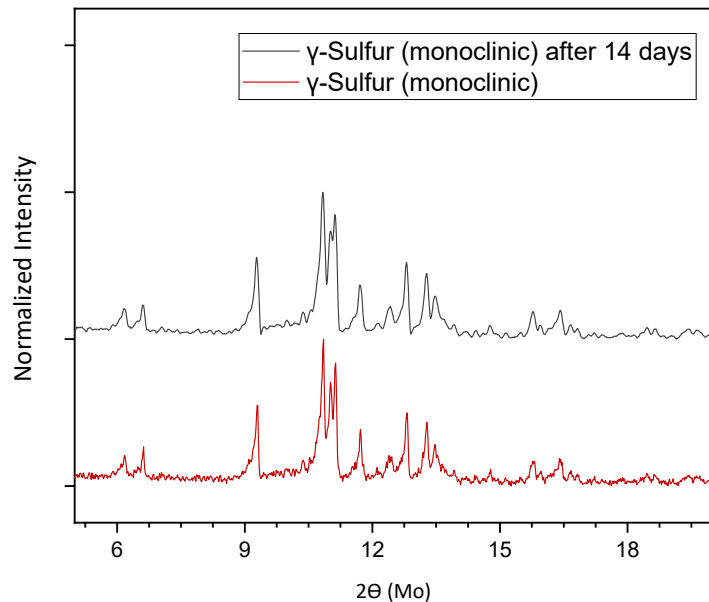
- Different OCV
- Different discharge/charge profile
- Better capacity retention



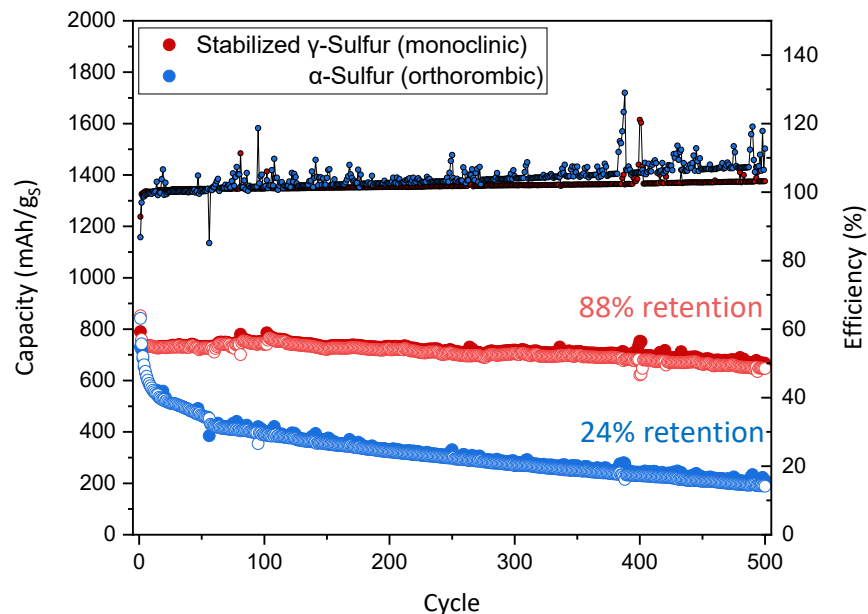
Sulfur content: **88%** ; Mass loading: **8 mg(S)/cm² @C/10** ; E/S = **5ml/g(S)**
Coin cell level Aprotic organic based electrolyte

Control on the Sulfur Chemical Structuration

- Depending on the special treatment, the structural organization of Sulfur can be modified without heating.
- Stabilization of the different Sulfur allotropes over time
- Stabilization of the capacity with the stabilized γ -Sulfur



X-Ray diffraction patterns of the different stabilized Sulfur Matrix



Sulfur content: **85%** ; Mass loading: **3 mg(S)/cm² @1C**
Coin cell level Aprotic organic based electrolyte

Buffering the Volume Expansion

- Depending on Sulfur density, up to 70% of volume expansion upon discharge

 Pulverization of the electrode along cycling

Our IP is not yet protected on this area, but ..

What about Sulfur density?

Summary

High energy density

Organized Porosity
→ Low E/S ratio

Artificial e⁻ Network
→ High Utilization
→ High mass loading

Long cycle life

„Fishscale coating“
→ Trapping of Li-pS

Volume Buffer
→ Prevent pulverization

- Monolithic „Sulfur Wafer“ with tailored **porosity** and **artificial percolation network**
- On this is applied a „**Fishscale**“ coating chemically bound to Sulfur thank to special treatment
- **prevent the Li-pS shuttle/dissolution** by of stabilization different allotropes, but also enhance the **electronic conductivity**
- Control the Sulfur density to accomodate the volume variation

Thank you for your attention

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