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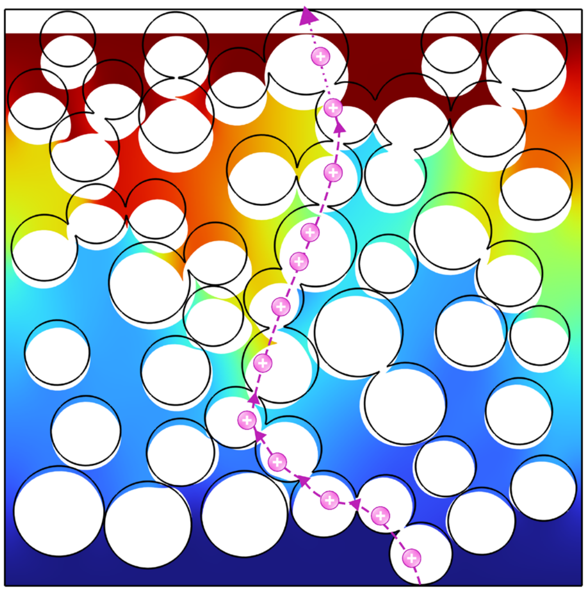

Numerical Simulation of the One-Way Mechanical-Electrochemical Coupling in Structural Supercapacitors

D. Peyrow Hedayati, G. Kahlmeyer, M. Kucher, R. Böhm
Leipzig University of Applied Sciences (HTWK), Leipzig, Germany
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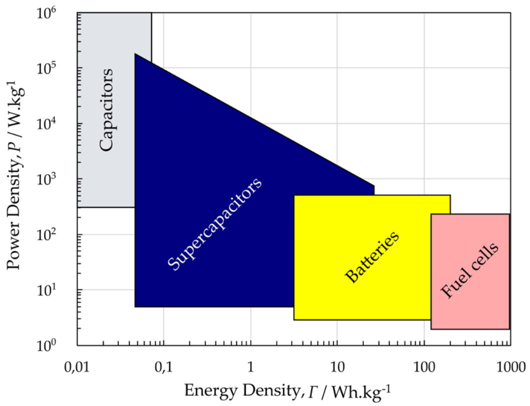
Table of Content

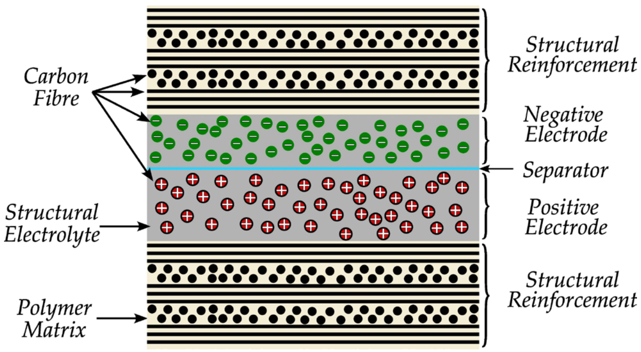
Multifunctional Energy Storage Composites

- Multifunctional Energy Storage Composite (MESC) carry load and store energy simultaneously.

[D. Peyrow Hedayati, ICCM23 Conf. Proc.]

- Examples: Structural Battery (SB) and Structural Supercapacitor (SSC)



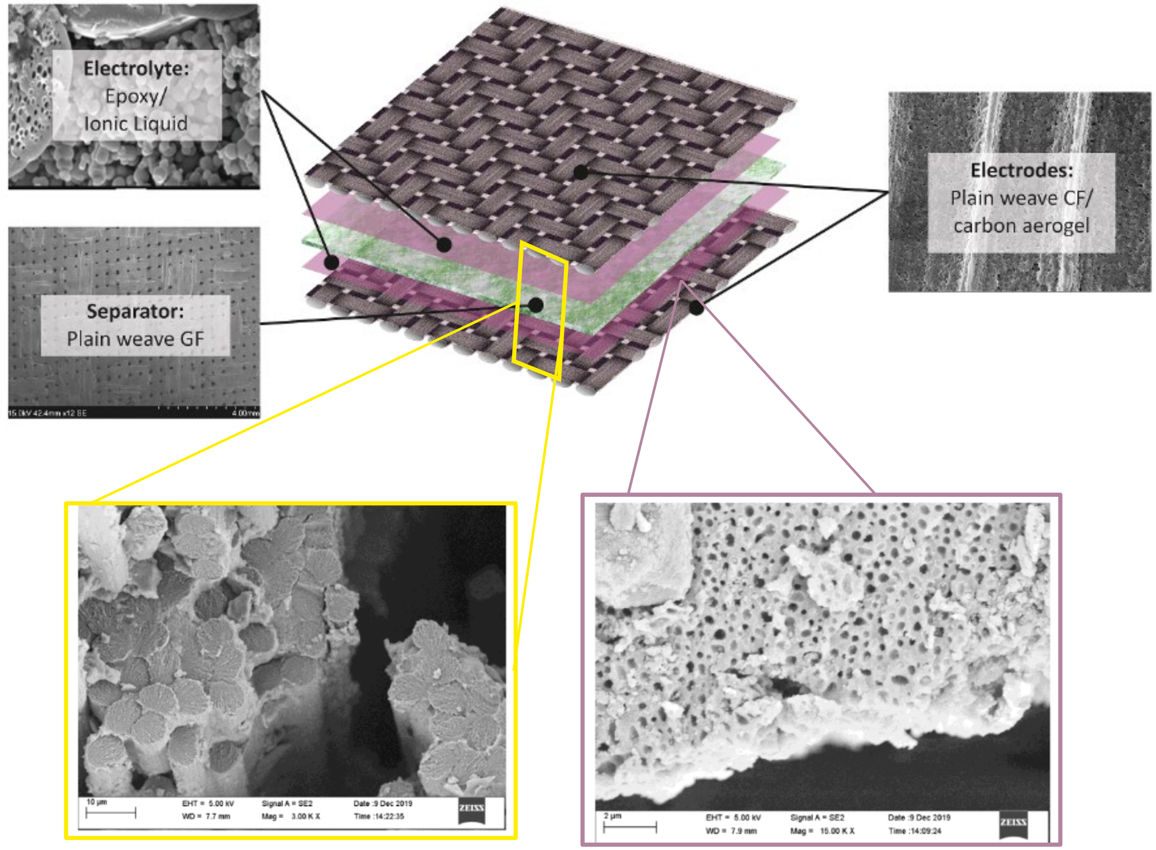


- High power density (SSC) for fast charge/discharge applications

Structural Supercapacitors
Architecture

SSC components:

- Electrode (CF)
- Structural Electrolyte
- Separator

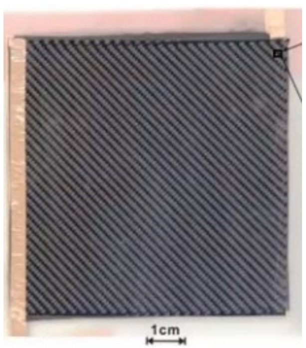


SSC composite

SSC matrix

[M.F. Pernice *et al* 2022 *Multifunct. Mater.* **5** 025002]

SSC demonstrator



[E. S Greenhalgh (2023, October 6), *Structural power composites - the route to more electric aircraft*]

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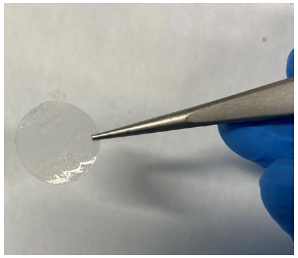
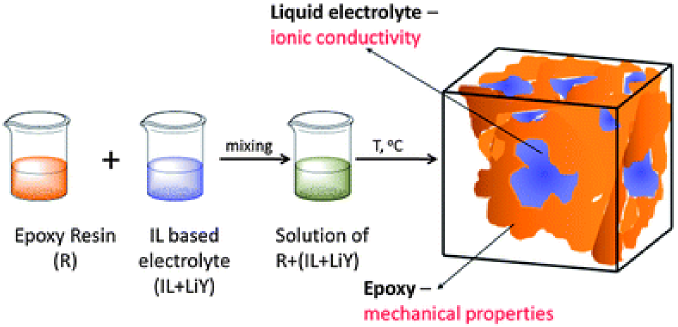
Structural Electrolytes

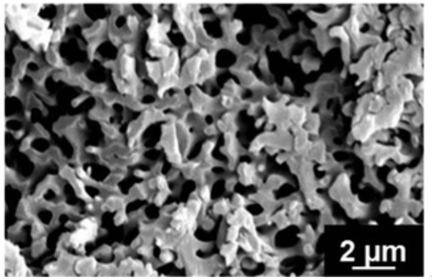
- Structural electrolytes: *ionically conductive* + *high mechanical integrity*
- Gel polymers are typically used but not stiff for structural applications.



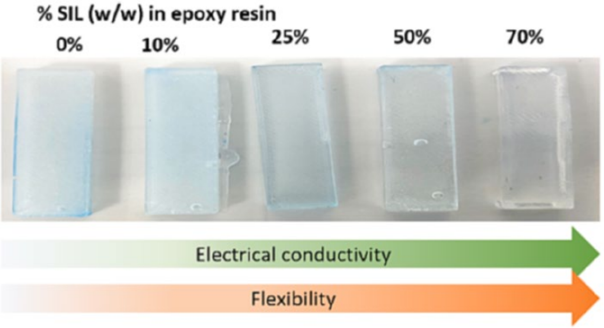
[*D. Peyrow Hedayati, Materials* 2023, *16*(3), 1232]

- Novel solution: **bicontinuous porous polymer electrolytes**
  - Porous polymer skeleton: non-conducting and stiff
  - Ionic liquid: ion conductive





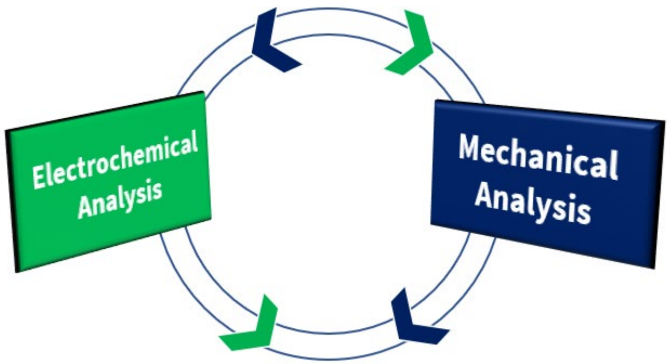
[Shirshova, J. Mater. Chem. A, 2013, 1, 15300-15309]



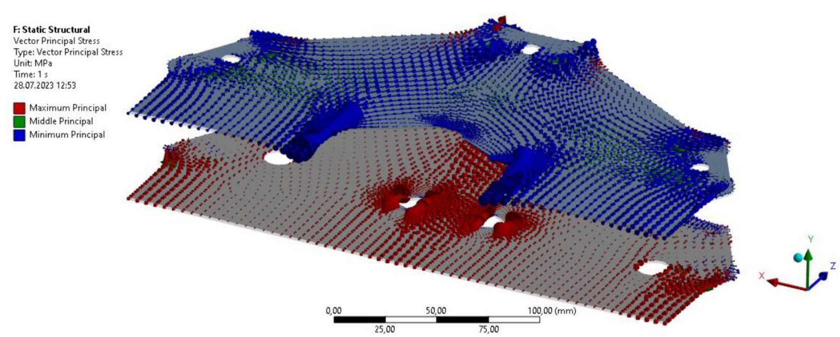
[Dharmasiri, CEJ, V.455, P.2, 2023, 140778]

Motivation and objective

- Multiphysics in a SSC



- SSCs as structural parts need to sustain mechanical loads.

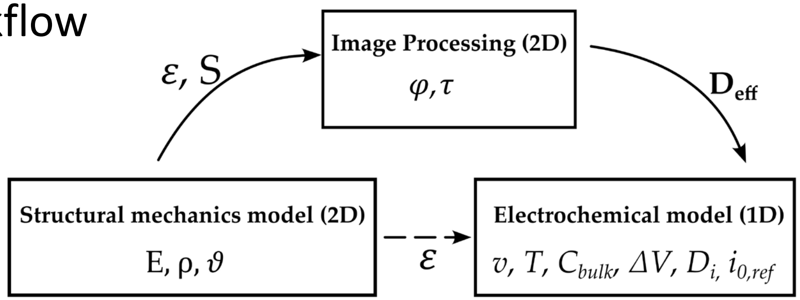


- How will the SSC electrochemical performance change under load conditions?

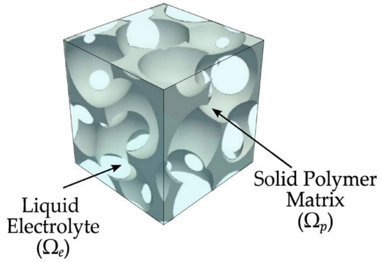
need for a mechanical-electrochemical model!

Methodology

- Modeling workflow

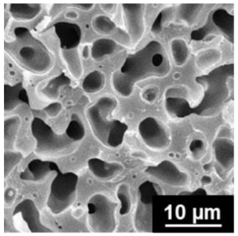


- Computational homogenization

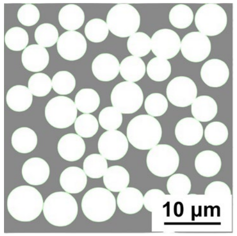


[Tu, 2020 *Multifunct. Mater.* 3 025001]

RVE



numerical regeneration



Electrolyte sample

SEM image microstructure

inverse bead model

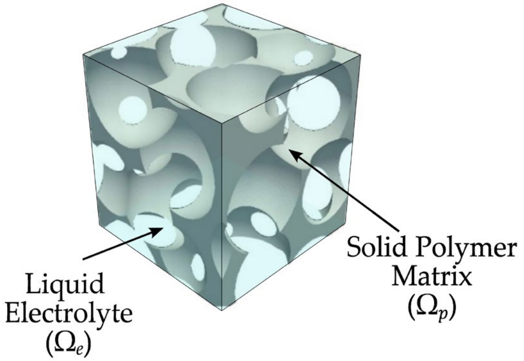
Governing equations

2D Linear Elastic Model (in $\Omega_p \times \mathbb{R}^+$)

$$\nabla \cdot \boldsymbol{S} + \boldsymbol{F}_V = 0$$

$$\boldsymbol{\varepsilon} = \frac{1}{2}\left[\nabla \mathbf{u} + (\nabla \mathbf{u})^T\right]$$

$$\mathbf{S} = \mathbf{C} : \boldsymbol{\varepsilon}$$



[Tu, 2020 *Multifunct. Mater.* **3** 025001]

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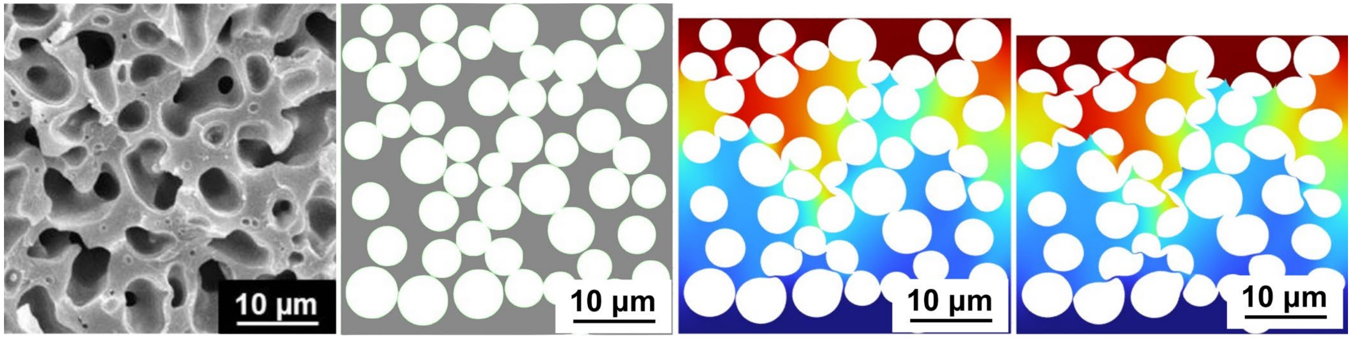


SEM image of the bicontinuous SPE | inverse bead RVE | deformation plots at ε=5%, and ε=10%

Governing equations

2D Linear Elastic Model (in $\Omega_p \times \mathbb{R}^+$)

$$\nabla \cdot \boldsymbol{S} + \boldsymbol{F}_V = 0$$

$$\boldsymbol{\varepsilon} = \frac{1}{2}[\nabla \mathbf{u} + (\nabla \mathbf{u})^T]$$

$$\mathbf{S} = \mathbf{C} : \boldsymbol{\varepsilon}$$

one-way coupling?

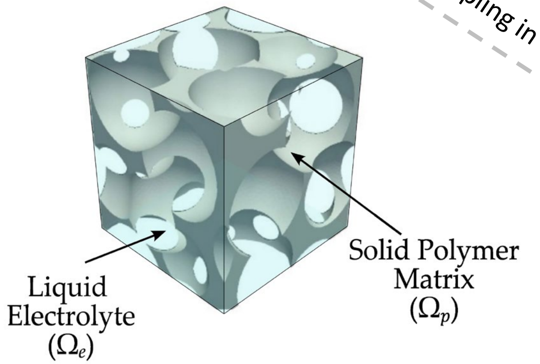
direct coupling in COMSOL?

1D Electro-Diffusion CV Model (in $\Omega_e \times \mathbb{R}^+$)

$$\phi_l = 0$$

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial c_i}{\partial x}$$

$$i_{\mathrm{loc}} = nFk_0(c_A \exp(\frac{(n-\alpha_c)F\eta}{RT}) - c_B \exp(\frac{-\alpha_c F\eta}{RT}))$$



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Governing equations

python™ ImageJ Image Processing and Analysis in Java

2D Linear Elastic Model (in $\Omega_p \times \mathbb{R}^+$)

$$\nabla \cdot \boldsymbol{S} + \boldsymbol{F}_V = 0$$

$$\boldsymbol{\varepsilon} = \frac{1}{2}[\nabla \mathbf{u} + (\nabla \mathbf{u})^T]$$

$$\boldsymbol{S} = \mathbf{C} : \boldsymbol{\varepsilon}$$

Diffusion (in $\Omega_e \times \mathbb{R}^+$)

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial c_i}{\partial x} \qquad \varphi = \frac{A_{pore}}{A_{total}}$$

$$D_{\hat{c}} = \kappa D_{:\,MC}$$

$$\kappa = \frac{\varphi}{\tau} \qquad \tau = \frac{L_g}{L}$$

1D Electro-Diffusion CV Model (in $\Omega_e \times \mathbb{R}^+$)

$$\phi_l = 0$$

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial c_i}{\partial x}$$

$$i_{\text{loc}} = nFk_0\left(c_A \exp\left(\frac{(n-\alpha_c)F\eta}{RT}\right) - c_B \exp\left(\frac{-\alpha_c F\eta}{RT}\right)\right)$$

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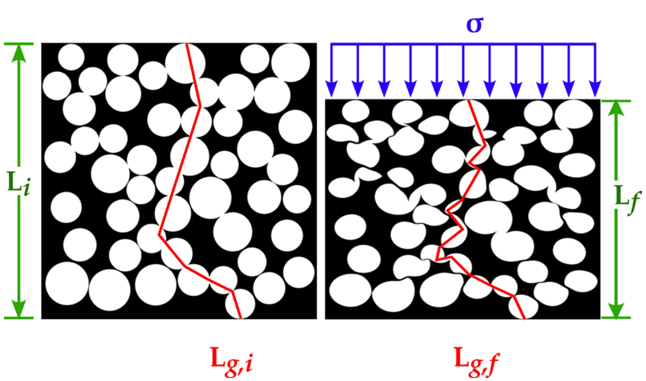

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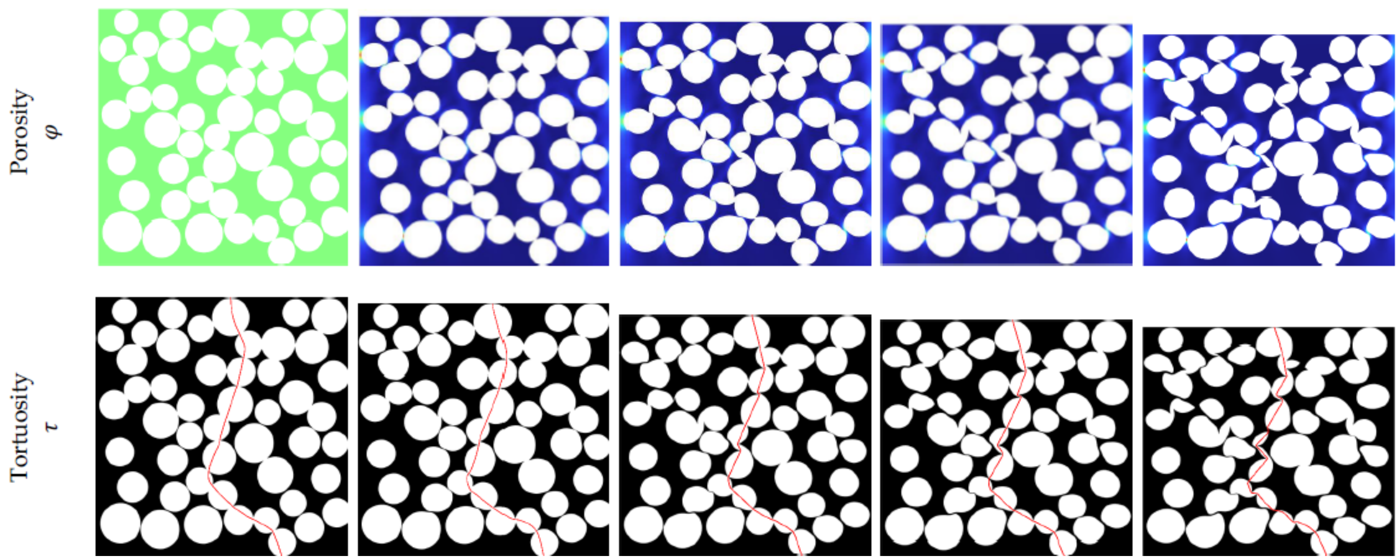
Results and Discussion

Compression Strain
low ⟷ high

Porosity
high ⟷ low

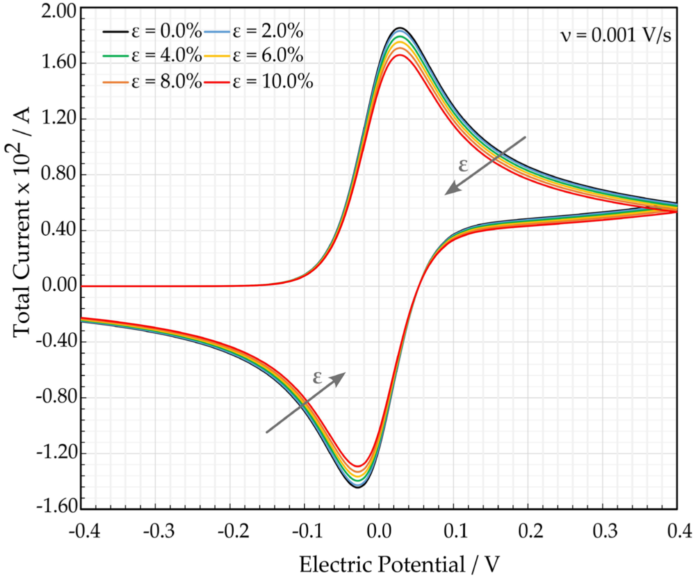
Tortuosity
low ⟷ high

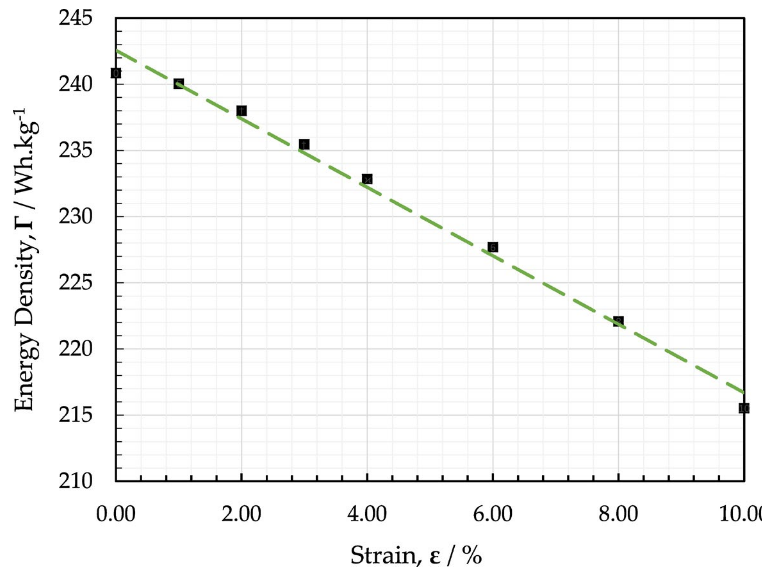


Effective Diffusion
high ⟷ low

Results and Discussion

Compressive strain leads to morphological changes in SE →
effective diffusion reduction →
lower specific capacitance (shrinking CVdiagrams)





increasing the compression strains to 10%→ 12% reduction in SSC energy density!

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Conclusion

- Structural supercapacitors as game changers for future lightweight high-power applications.
- Proposition of a model to investigate the mechanical-electrochemical coupling in a structural supercapacitor with a bicontinuous polymer electrolyte.
- A one-way coupling introduced using FEA and image processing techniques.
- The results showed that increasing the compressive strains up to 10% lowers the energy density of the SSC by around 12%.
- Future efforts will focus on validating the model with experimental data.

Research Team

Leipzig University of Applied Sciences (HTWK)

Composite Lightweight Engineering Group

Head of group
Prof. Dr. Robert Böhm

Group leader
Dr. Michael Kucher

Research Associate
Davood Peyrow Hedayati

Undergraduate student
Gabriel Kahlmeyer

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M-era.Net PRINTCAP

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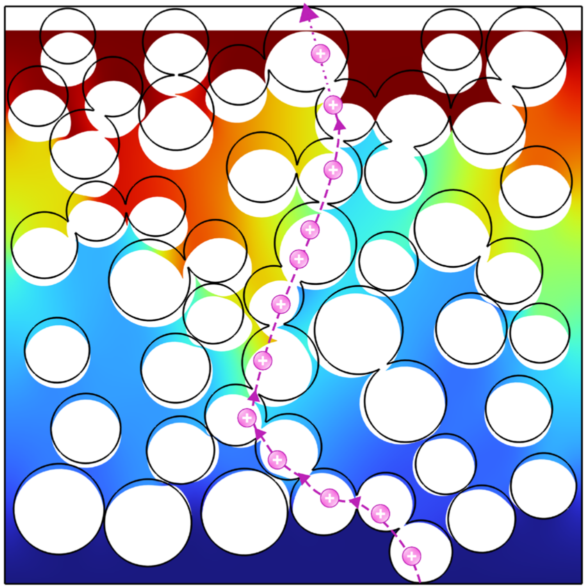
Thank you for your attention!

M.Sc. Davood Peyrow Hedayati
Research Associate
Faculty of Engineering
Leipzig University of Applied Science

davood.peyrow_hedayati@htwk-leipzig.de



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