Understanding the Influences of Laser Perforation on Thick Electrodes for Lithium Ion Batteries via 3D Microstructure Simulations

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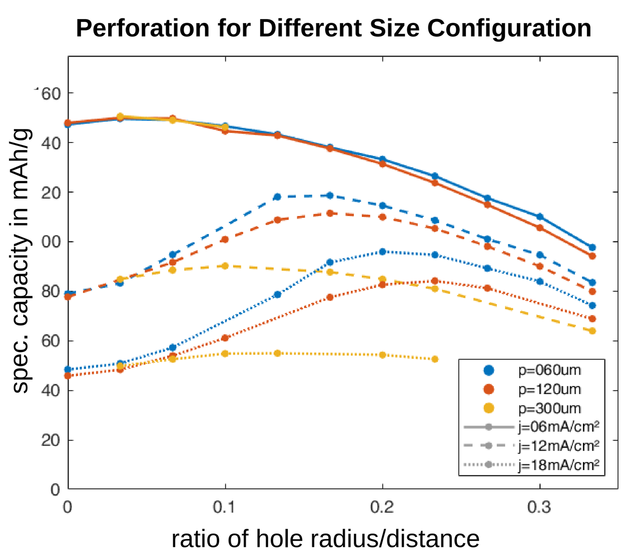
Motivation & Approach

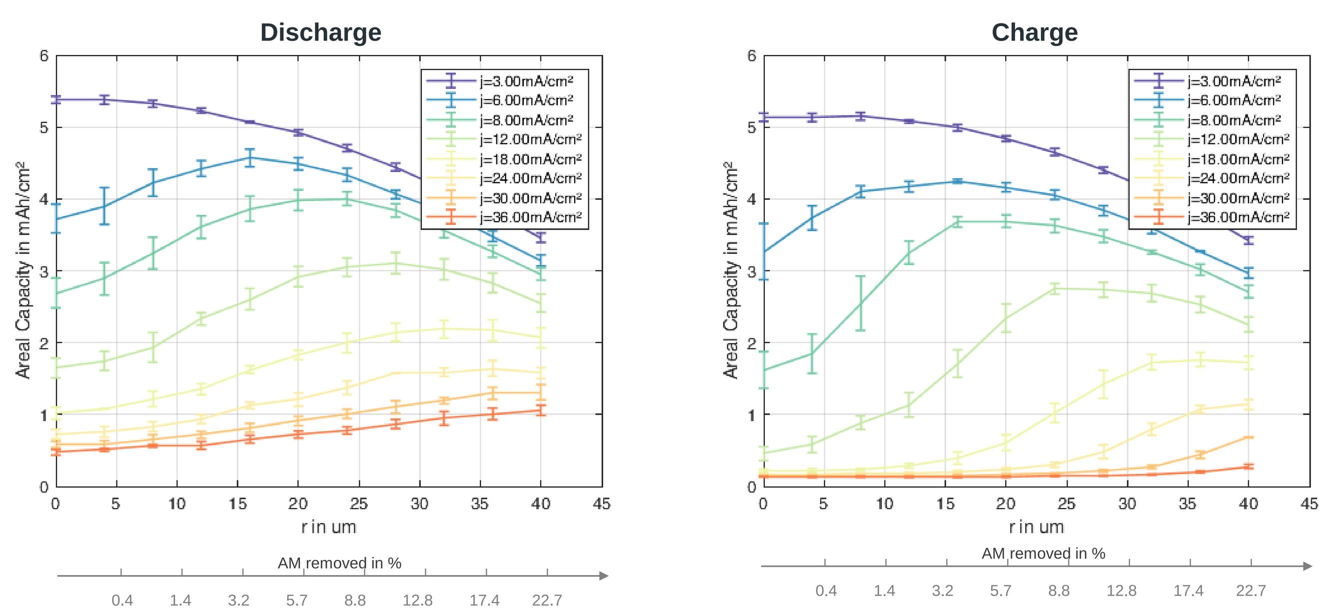
- **Thick electrodes** provide high energy densities, but suffer from **ionic diffusion limitations.**
- **Laser perforation** selectively **removes material** with spatial precisions of tenth of micrometers, thereby creating ion diffusion channels.
- The 3D-microstructure resolved simulation tool BEST[1] is used to determine the **optimal trade-off between** the competing factors of **capacity loss** and **increase in ion conductivity** due to material ablation.

Simulation Results



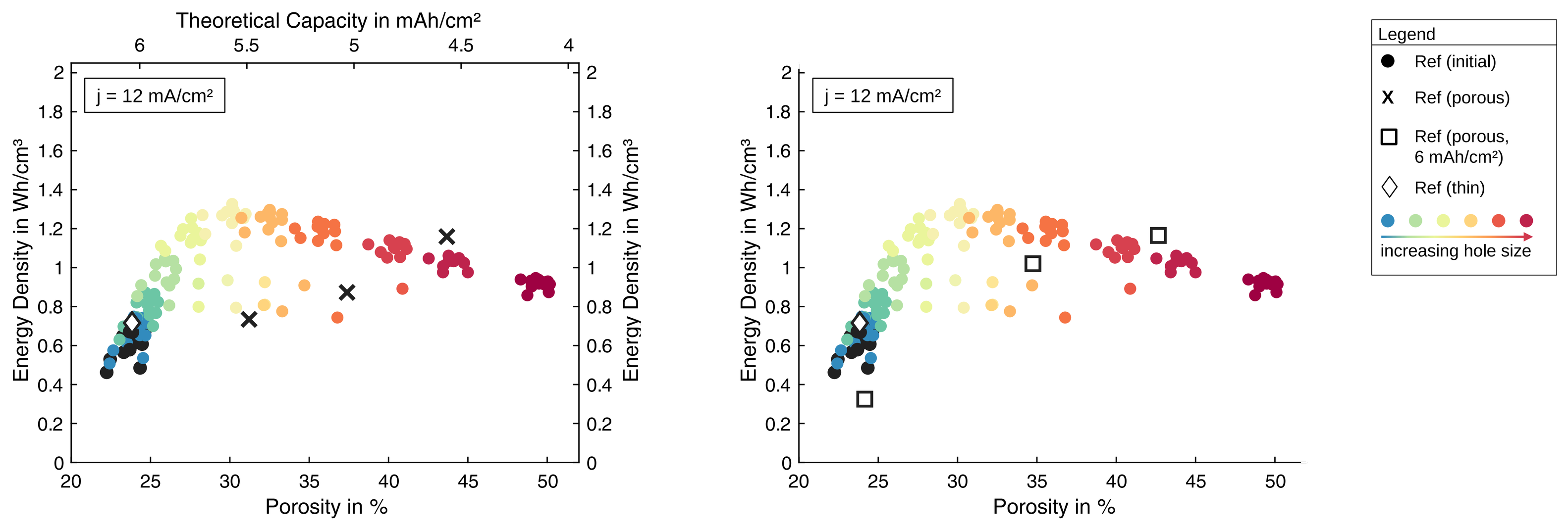
Setup
NMC$_{622}$
Q_{init} = 6mAh/cm²
ε_{init} = 24%
d = 105µm

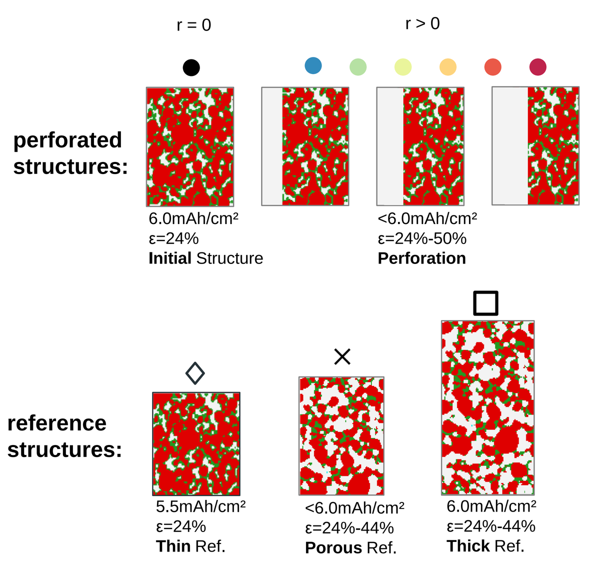
- Optimal ablation of active material: 5%-10%
- Preferably, hole radius as small as possible
- Minimal hole radius is limited for real perforation setups
- System can be optimized depending on specific operation current



const. hole distance
p = 120µm

Perforation vs. Homogeneous References



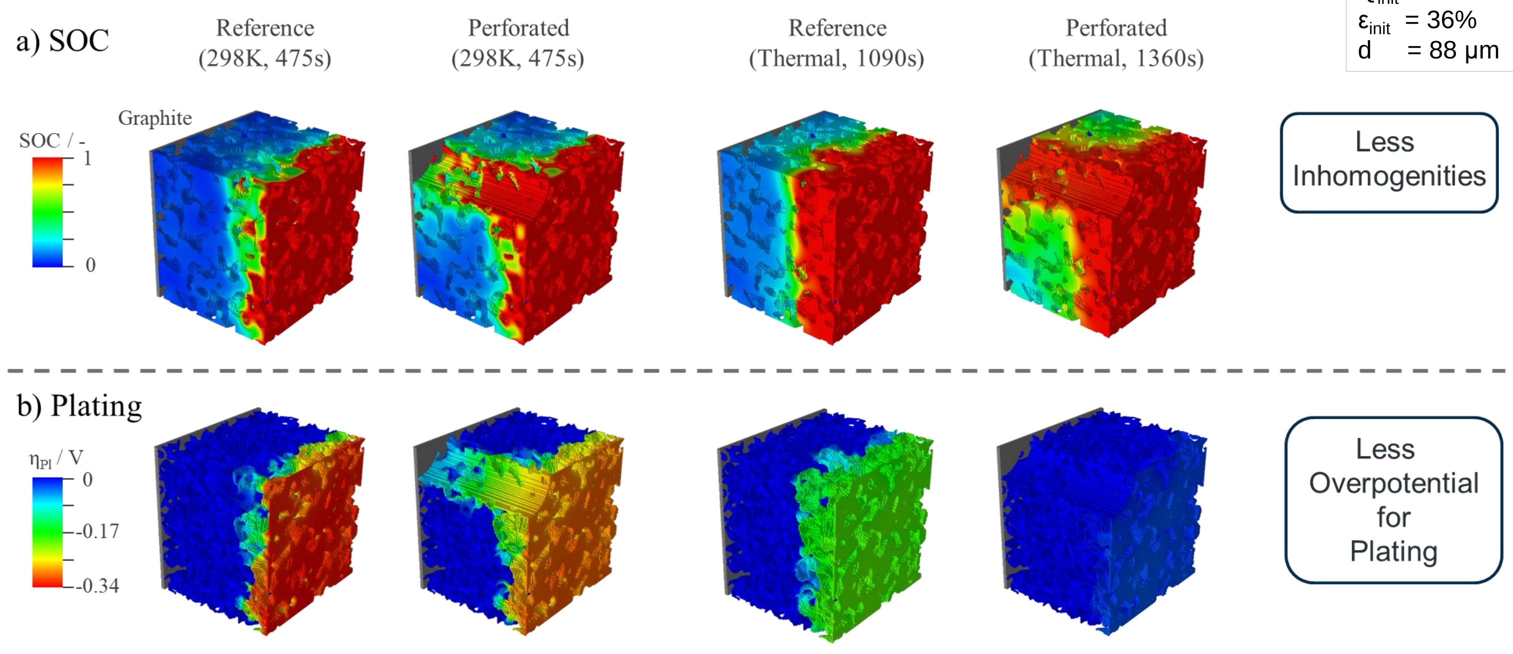


- Comparison with a thinner and other more porous references shows: The **inhomogeneous perforation** structure performs **better** than **homogeneous reference** structures
- Concluding: Not the additional electrolyte reservoir, but rather the inhomogeneous **diffusion channels are the significant factor** to the improvement of the rate capability

Perforation on Plating

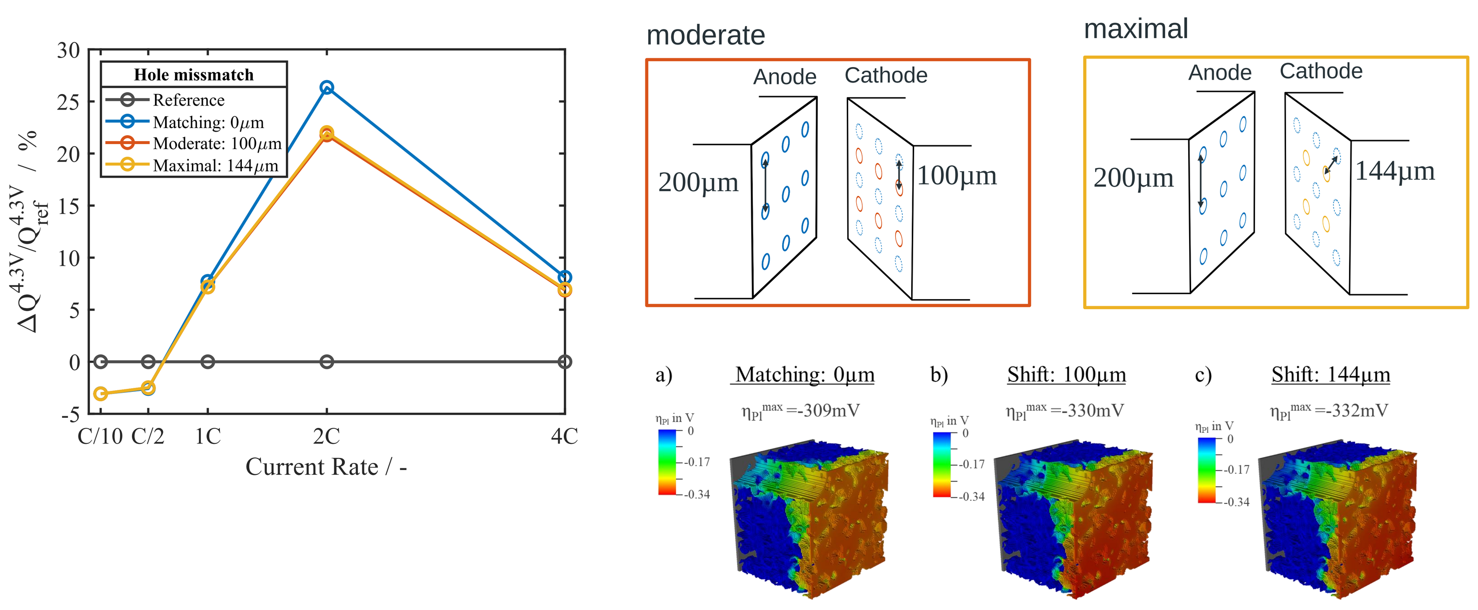
[2]

Setup
Graphite
Q_{init} = 4.2mAh/cm²
ε_{init} = 36%
d = 88 µm



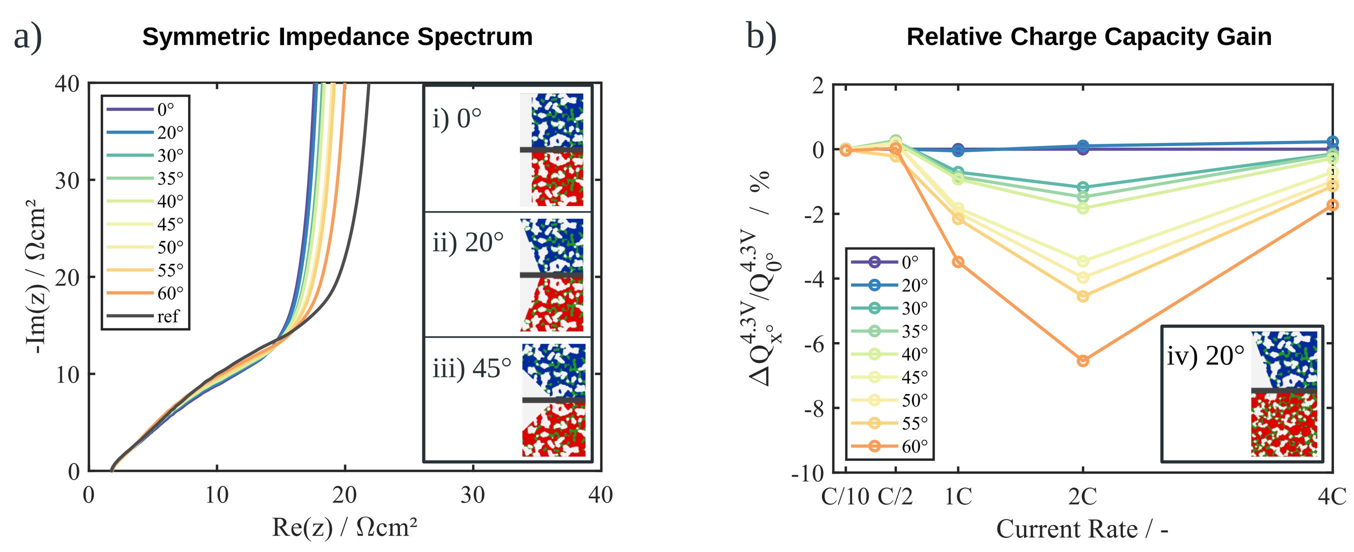
- Perforated structures show more homogeneous SOC distribution and thus a greater utilization of the active material
- This leads to a reduction in plating risk for perforated graphite for 2C
- Thermal simulation suggest even no plating risk (η_{Pl} > -30mV) when accounting for heat evolution during charging

Spatial Misalignment



- The effect of misalignment on the charging performance is moderate
- Here it reduces the beneficial effect of perforation by 5% at 2C
- For plating: no significant influence is observed

Influence of the Hole Shape



- In manufacturing, cone shaped holes are fairly common in contrast to perfect cylindric shapes.
- Simulated pore transport increases only significantly for holes with entrance angles of >20°
- A small entrance angle can even be beneficial for the retained charge capacity

References:

(1) Battery and Electrochemistry Simulation Tool: https://www.itwm.fraunhofer.de/en/departments/sms/products-services/best-battery-electrochemistry-simulation-tool.html

(2) De Lauri, V.; Krumbein, L.; Hein, S.; Prifling B.; Schmidt V.; Danner, T.; Latz, A. et al., *ACS Appl. Energy Mater.* **2021**, 4, 13847-13859.

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Conclusion

- Optimal perforation configurations depend on the specific operation.
- In general as small structures as possible lead to better results.
- Optimal ablation fractions are ca. 5%-10% of the active material .
- Typical manufacturing errors, on hole shape and alignment do not lead to a major reduction in performance.

GEFÖRDERT VOM Bundesministerium für Bildung und Forschung

HIU HELMHOLTZ INSTITUTE ULM Electrochemical Energy Storage

DLR Deutsches Zentrum für Luft- und Raumfahrt German Aerospace Center

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