PAUL SCHERRER INSTITUT

ELECTROCHEMISTRY LABORATORY

BATTERIES

Heraeus

Characterization of Porocarb–Si Composite Material for Negative Li-ion Battery Electrodes

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Introduction

Graphite's theoretical specific charge is 372 mAh/g:

- it can deliver specific charge close to the theoretical one
- its improvement limits have been reached

Main disadvantages of silicon as electrode material are:

- Low intrinsic electronic conductivity
- Drastic (up to 400%) volume expansion upon lithiation
- Ever growing SEI

Combine advantages – avoid disadvantageous behavior!

New pre-commercial carbon–silicon composite, where Si embedded into the porous carbon structure.

Expectations:

- SEI is formed on carbon
- Stable cycling and high coulombic efficiency
- Specific charge higher than graphite's

Experimental

Mixing: carbon precursor & 100nm size Si nanoparticles

Homogenising by melting

Infiltration into silica matrix

→ Carbonization

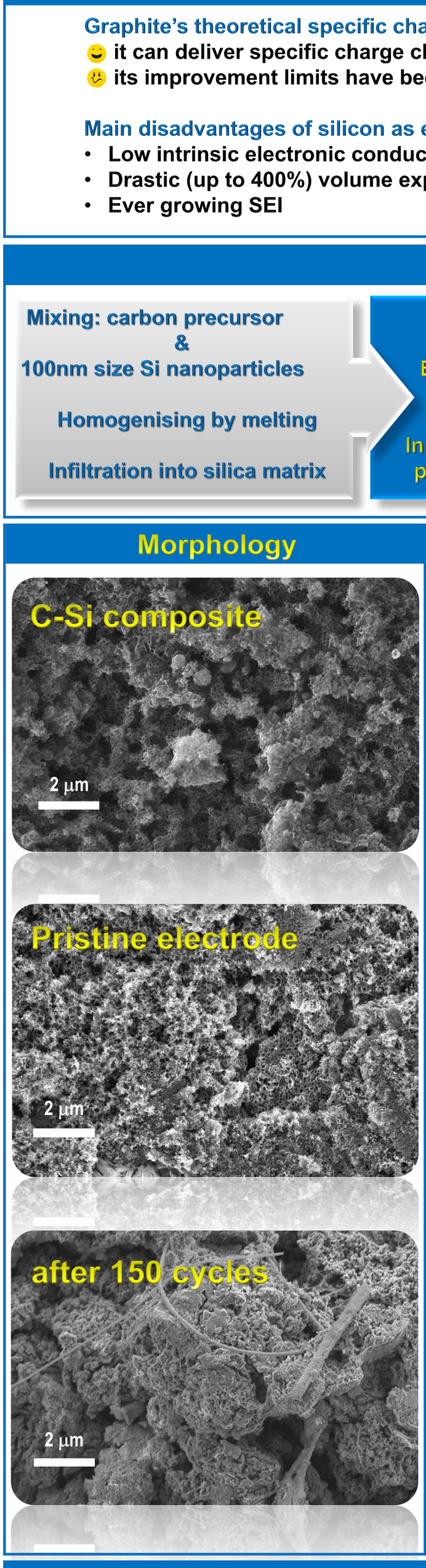
→ Etching of template

→ Inner porosity of C–Si particles is exposed

→ Porocarb-Si Composite

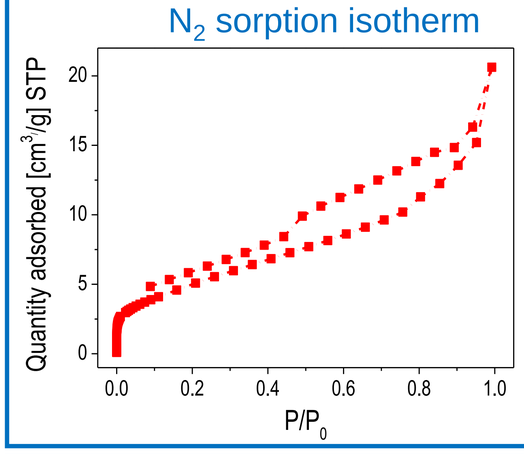
- **Composite:** 20 % silicon, 80 % carbon
- **Electrode:** 80 % C-Si composite, 10 % Super P, 10 % PVDF
- **Electrolyte:** LP30 (1 M $LiPF_6$ in EC:DMC)
- Coin-type cell, Li counter electrode
- **Cycling:** C/10 = 420 mA/g and 1C = 4200 mA/g of Si
- **CV:** 0.005 mV/s between 0 and 1 V vs. Li^+/Li

Morphology

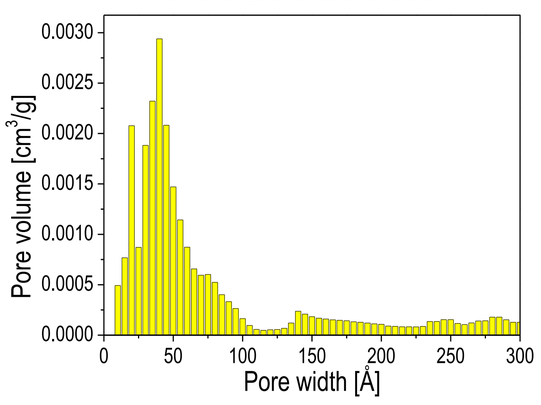


Gas adsorption

N_2 sorption isotherm



Pore size distribution

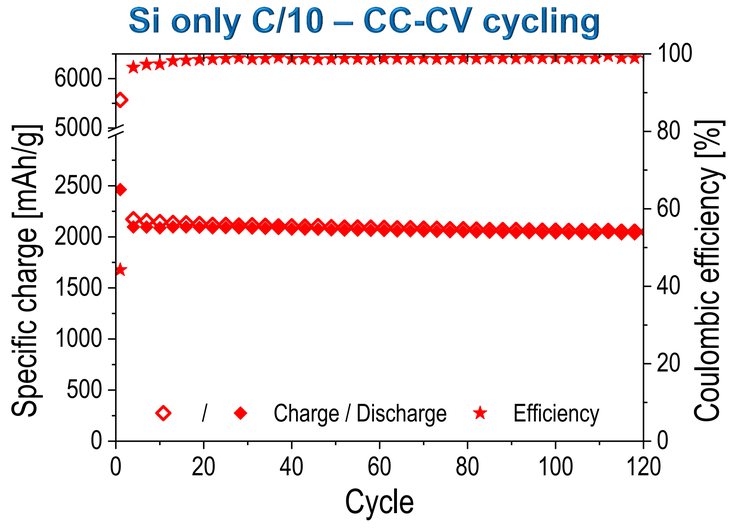


- N_2 was used as adsorbate
- Samples were degassed at 300°C for 16 h
- The sample amount was ~0.2 g
- The isotherm evaluated by BET method
- The pore size distribution, pore volume, and pore size – by DFT method

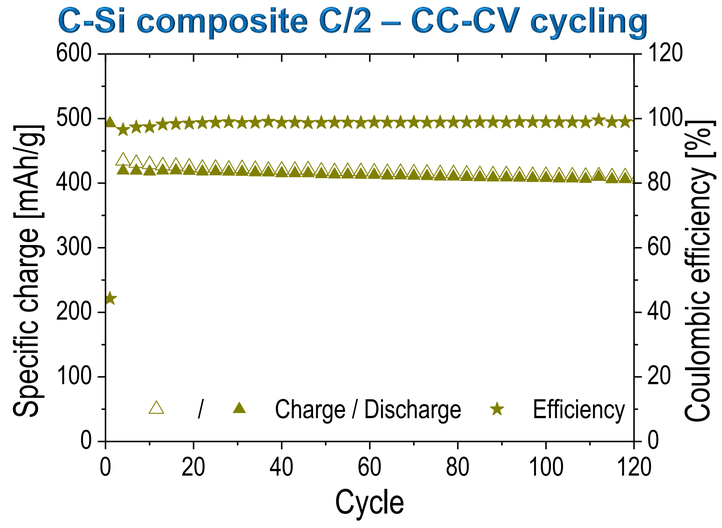
- **Specific surface area: 17 m^2/g**
- **Total pore volume: 0.024 cm^3/g**
- **Average pore size: 52 Å**

Electrochemical tests

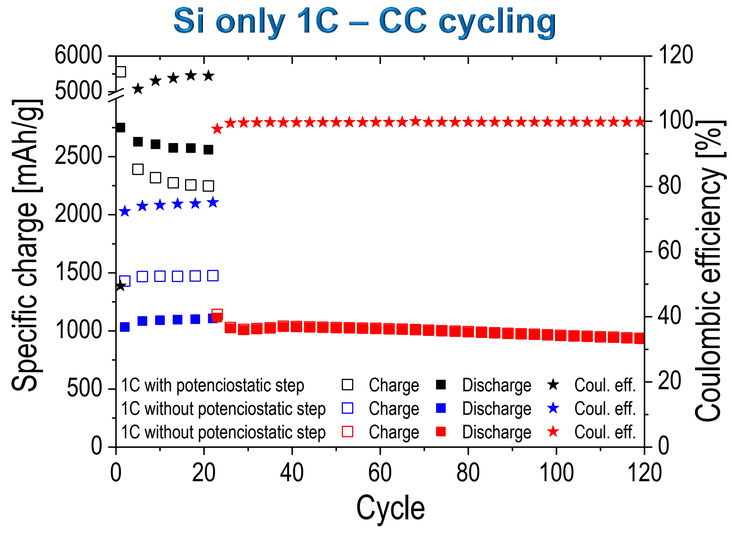
Si only C/10 – CC-CV cycling



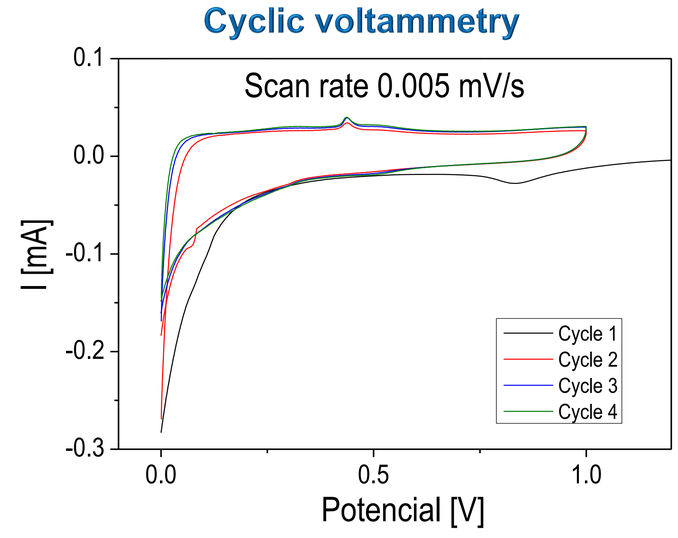
C-Si composite C/2 – CC-CV cycling



Si only 1C – CC cycling



Cyclic voltammetry



Conclusions and outlook

- High and stable specific charge for more than 100 cycles at C/10 with no set specific charge limits applied
- SEI presumably on carbon

Porocarb–Si R&D material:

- carbon host with lower surface area – to mitigate low initial coulombic efficiency
- structural in-situ XRD and X-ray tomography - to understand long term cycling stability