PAUL SCHERRER INSTITUT

ELECTROCHEMISTRY LABORATORY

BATTERIES

Surface investigation of 30nm amorphous Si thin films cycled as negative electrode for Li-ion batteries

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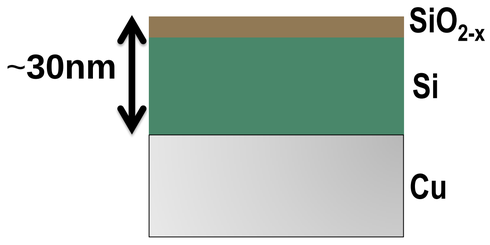
Motivation

- **Electrochemical** and **surface analysis** (XPS) of 30nm amorphous phosphorus doped (n-type) Si thin films (used as model material)
- Understand the properties of the **solid electrolyte interphase (SEI)** growth and **Li-Si alloy** formation upon lithiation/delithiation

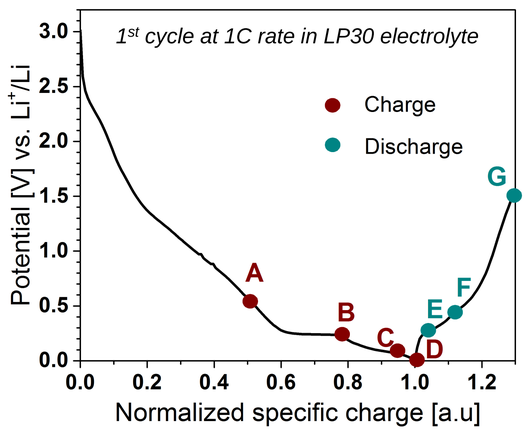
Model material:
30nm P-doped Si thin film on Cu (PECVD deposition)

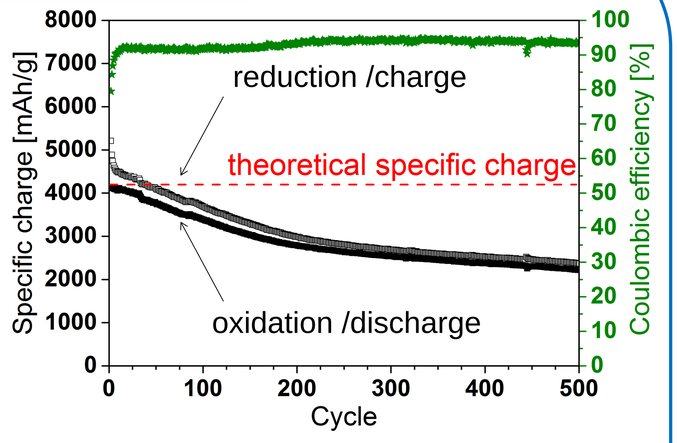
- No binder, no conductive agent



Electrochemical performances

Galvanostatic profile



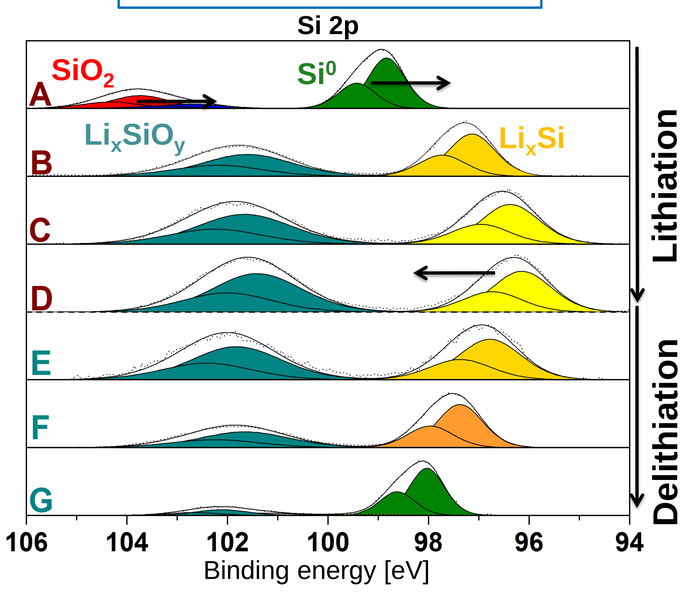


→ **Theoretical** specific charge (ca. 4000 mAh/g) achieved in the **first 20 cycles**

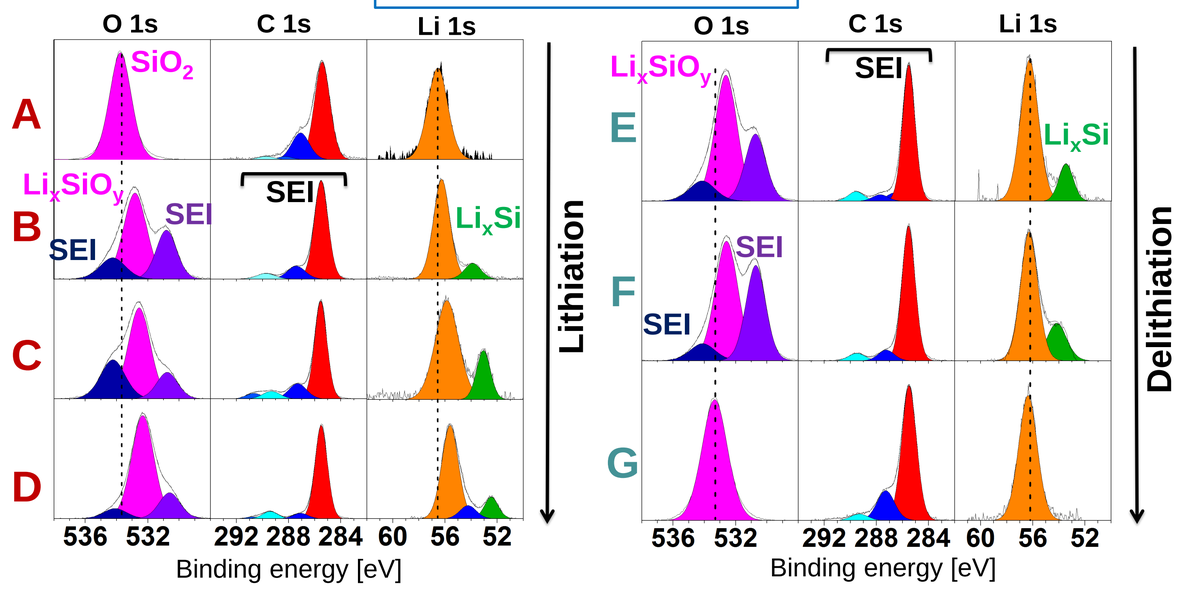
→ **50% specific charge** maintained for **500 cycles**

Post mortem XPS investigation

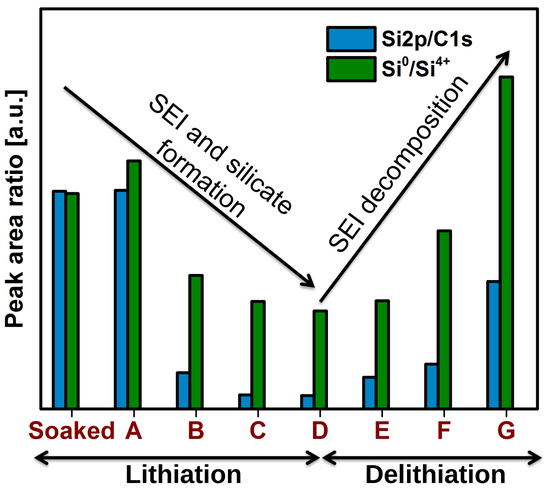
Li-Si reaction



Surface evolution



SEI and SiO_2 evolution



Charge

A → No SEI formation, no reaction involving silicon

B-D → SEI growth, Li-silicate and Li-Si alloy formation

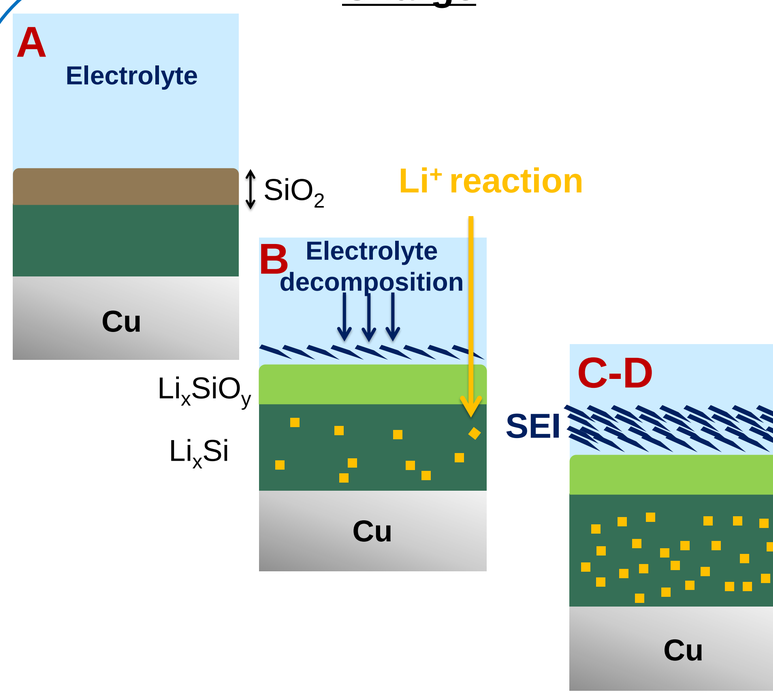
Discharge

E-G → Reversible Li-Si de-alloying, SEI removal, partial Li-silicate dissolution

- Breathing effect of the SEI
- SiO_2 thickness reduced after the first discharge

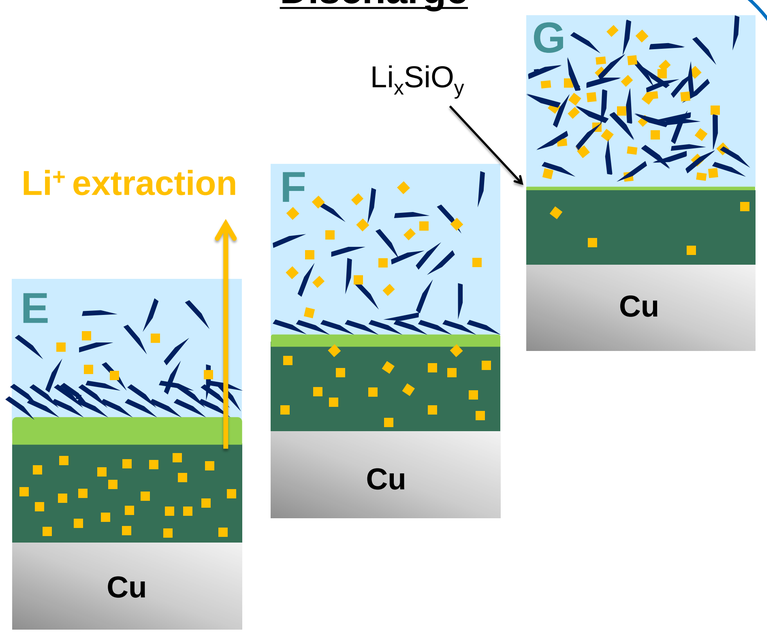
Reaction mechanism

Charge



- Si^0 and SiO_2 → Li-Si and Li-silicate compounds
- **SEI** (organic/inorganic) formation at potential **lower than 0.6V**

Discharge



- Li_xSi delithiated to Si^0
- **Irreversible** lithiation mechanism for **SiO_2**
- Li-silicate thickness is reduced
- **SEI decomposition** and **dissolution**

Conclusions

- **High stability** of Si thin films during cycling
- Specific charge retention up to **50%** of the **initial value after 500 cycles**
- In-house XPS on **Si 2p**, **C 1s**, **Li 1s** and **O 1s core levels** to monitor SEI and Li-Si alloy
- **SEI** forms only at potential **lower than 0.6V**
- Elucidation of the **SEI growth mechanism** and **Li-Si alloy formation** during the **early stages of cycling**

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