



Fabian Single, Birger Horstmann and Arnulf Latz

Modelling Solid Electrolyte Interphase growth, a Novel Description of Porous Layer Evolution



DLR

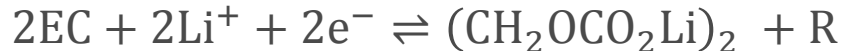
**Deutsches Zentrum
für Luft- und Raumfahrt**
German Aerospace Center
Institute of Engineering Thermodynamics
Computational Electrochemistry

Solid Electrolyte Interphase (SEI)

Formation

- Reduction of electrolyte, e.g.

Ethylene Carbonate (EC)

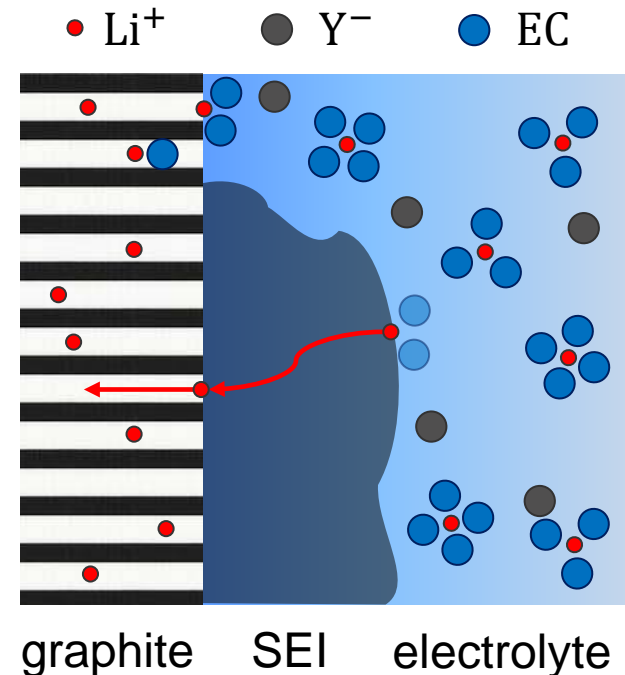


SEI advantages

- Almost **no further electrolyte reduction**
- Protection of graphite from exfoliation
- Increase in mechanical stability of graphite

SEI disadvantages

- Li⁺ ion consumption
 - Continuous growth
 - Increase in impedance
- } **capacity fade**



Reviews on SEI composition:

- Agubra, V. a., & Fergus, J. W. *Journal of Power Sources* **268**, 153–162 (2014).
- Verma, P., Maire, P., & Novák, P. *Electrochimica Acta* **55**(22), 6332–6341 (2010).

SEI Modeling - Literature Review

Current models – zero dimensional

- **Homogeneous** composition
- **Single** transport mechanism
- Fast reaction kinetics
- Single reaction interface

transport-limited growth

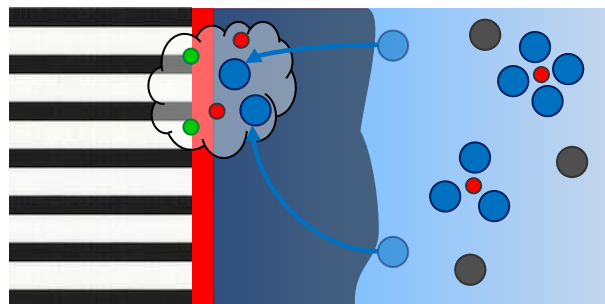
$$L(t) \propto \sqrt{t}$$

Solvent/anion diffusion:

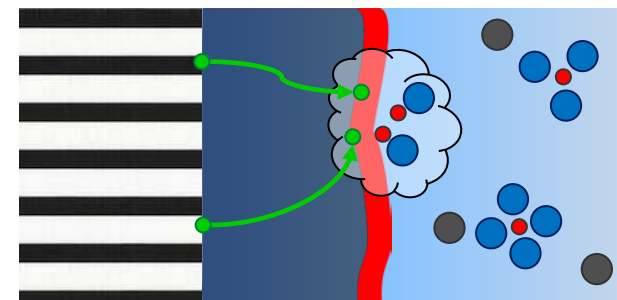
- Pinson, M.B. & Bazant, M.Z. *Journal of the Electrochemical Society* **160**, A243-A250 (2012).
- Ploehn, H.J., Ramadass, P. & White, R.E. *Journal of The Electrochemical Society* **151**, A456 (2004).

Electron conduction:

- Christensen, J. & Newman, J. *Journal of The Electrochemical Society* **151**, A1977 (2004).



• Li⁺ • Y⁻ • EC • e⁻



graphite SEI electrolyte