An electrochemo-mechanical coupled model for lithium ion batteries

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Introduction

Lithium ion batteries are the industry choice for energy storage in electric vehicles. A study on the electrochemo-mechanical coupled behaviour of lithium-ion batteries has been carried out accounting for stresses across the electrode and non-linear diffusion using a P2D and physics based equivalent circuit model. The results can provide insights to inform improved battery control algorithms for longer lifetimes.

Mechanical model

A stress model for a single spherical electrode particle has been proposed by Zhang et al. [4]. The radial and tangential stresses and displacement caused by lithium (de)intercalation into electrode particles are respectively

$$\sigma_r(r) = \frac{2\Omega E}{3(1-v)}\left(\frac{1}{R_i^3}\int_0^{R_i}\bar{c}r^2\mathrm{d}r - \frac{1}{r^3}\int_0^{r}\bar{c}r^2\mathrm{d}r\right) \quad (1)$$

$$\sigma_\theta(r) = \frac{\Omega E}{3(1-v)}\left(\frac{2}{R_i^3}\int_0^{R_i}\bar{c}r^2\mathrm{d}r + \frac{1}{r^3}\int_0^{r}\bar{c}r^2\mathrm{d}r - \bar{c}\right) \quad (2)$$

$$u(r) = \frac{\Omega}{3}\frac{1+v}{1-v}\frac{1}{r^2}\int_0^{r}\bar{c}r^2\mathrm{d}r + \frac{2\Omega}{3}\frac{1-2v}{1-v}\frac{r}{R_i^3}\int_0^{R_i}\bar{c}r^2\mathrm{d}r \quad (3)$$

Volume variation by lithium (de)intercalation for the pouch cell can be estimated by

$$\mathrm{d}L_{\mathrm{int}} = n\cdot\sum_{i=1}^{n_p+n_n}\mathrm{d}L_i = n\cdot\sum_{i=1}^{n_p+n_n}\epsilon_s\Omega c_{i,\mathrm{avg}}L_i \quad (4)$$

P2D model

Lithium-ion batteries can be modelled by a pseudo-2D (P2D) model, where the entire cell is represented by 1D structure as shown in Figure 1. Governing equations have been mentioned by many other papers for battery modelling and are not repeated here, with full details given in Ai et al. [1].

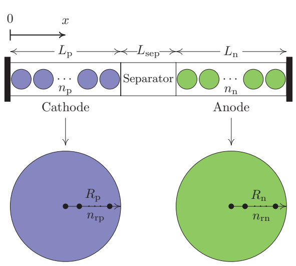

Figure 1: Schematic configuration of the P2D battery model.

Result 0 - Validation

The responses of voltage and thickness change for the Enertech SPB655060 pouch cell ($LiCoO_2$−graphite) under different discharge C-rates have been calculated and compared with experiments in Figure 2. The thickness change of the pouch cell is estimated by Equation 4 in the mechanical model. A characteristic plateau in the thickness change of the pouch cell is well predicted, by considering the volume change of the crystal structure of both electrodes, see Ai et al. [1] for more details.

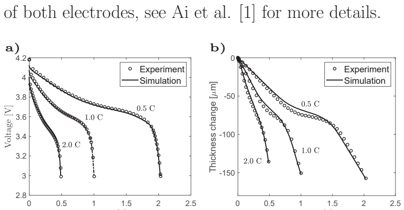

Figure 2: Validation of the model: (a) voltage and (b) thickness change of the pouch cell.

Result 1 - Stress Distribution

The distributions of the maximum tangential stress at particle surface under different C-rates (constant currents for cycling) are given in Figure 3. The magnitudes of tangential stresses generally increase with C-rate, and larger stresses can be found close to the separator. This behaviour can be explained by considering that the reaction current density between cathode and anode mainly occurs at particles close to the separator for high C-rates.

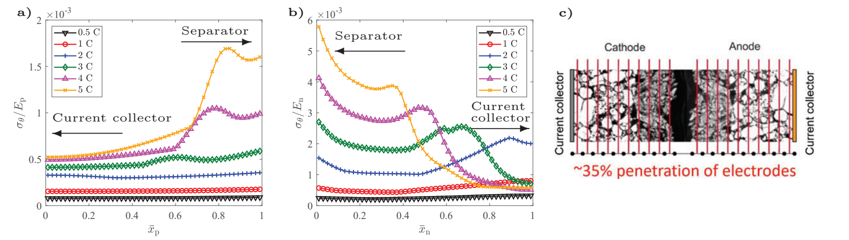

Figure 3: Maximum tangential stress at particle surface in electrodes at different C-rates of discharging: stress distribution in (a) cathode and (b) anode. (c) experimental obeservation of particle fragmentation close to the separator from Christensen [2];

Result 2 - SOC dependent diffusion

The diffusion coefficient of Li (Ds) in both electrodes is phase-dependent and varies as a function of the SOC during the operation. Figure 4 a and b show the half-cell OCVs and the variation of lithium diffusion coefficient with SOC for the Kokam 7.5Ah (SLPB75106100). The Ds is two orders of magnitude different at the anode graphite staging and at the phase transition of cathode NMC. A greater variation in tangential stress during discharge is observed when Ds (SOC) is accounted for as shown in Figure 5, indicating certain SOC windows suffer more mechanical damage.

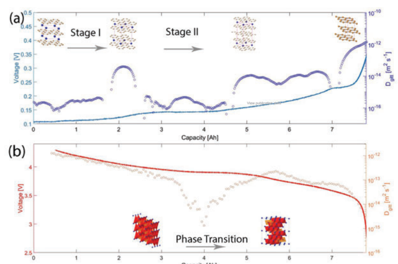

Figure 4: The diffusion coefficient determined by GITT and the OCV curve from the graphite/Li half cell in (a) and from the NMC/Li half cell in (b).

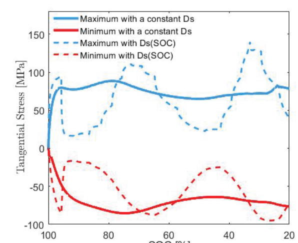

Figure 5: Maximum and minimum tangential stress generated during 1C discharge when Ds is considered as a constant (solid lines) and as a function of SOC (dotted lines).

Result 3 - Physics-inspired equivalent circuit model

Extending the single cell P2D-based calculations to a pack is computationally prohibitively expensive. A simplified but feasible approach is to convert the single particle model into a physics-inspired equivalent circuit model (PECM), in which ideal voltage sources, resistors and capacitors are used to represent the cell (see Figure 6 and [3]). Figure 7 shows the surface tangential stress in the anode particle during a simulated 2C discharge of two Kokam 5Ah cells connected in parallel for three temperature conditions. When the cell closest to the load point (C2) is colder than C1, the baseline trend of C2 delivering more current is reversed, and hence the stress is higher in C1. This is a useful tool to develop pack topologies that aim to maintain uniform degradation.

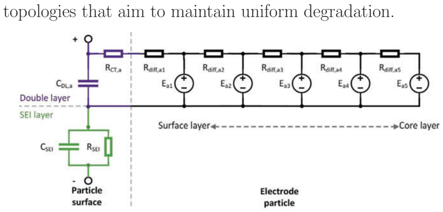

Figure 6: Schematic of one electrode in PECM [3].

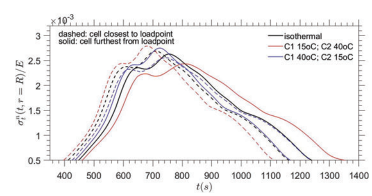

Figure 7: Surface tangential stress in the anode for two cells in parallel.

Conclusion

- Electrochemical-mechanical coupled P2D model for lithium-ion batteries.
- Large stresses close to the separator leading to particle fragmentation for high C-rates.
- SOC-dependence of diffusion coefficient has significant influence on stress generation and hence mechanical damage at phase transitions.
- The PECM for battery packs showing temperature effects on stress distribution over individual cells.

References

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