Supplementary Information (SI) for Journal of Materials Chemistry A.


# Supplementary Materials: Mechanical Abuse and Safety in Sodium-Ion Batteries

Bo Rui[1, 2], Shuguo Sun[1, 2], Xijun Tan[1, 2], Chanmonirath (Michael) Chak[3], Lin Ma[3*], Jun Xu[1, 2*]

[1]*Department of Mechanical Engineering, University of Delaware, Newark, DE 19716, USA*

[2]*Energy Mechanics and Sustainability Laboratory (EMSLab), University of Delaware, Newark, DE 19716, USA*

[3]*Department of Mechanical Engineering and Engineering Science, The University of North Carolina at Charlotte, Charlotte, NC 28126, USA*

**Table. S1** The discharge capacity for each cycle in conditional test and their average capacity

| | 1st cycle discharge capacity | 2nd cycle discharge capacity | Average |
|---|---|---|---|
| Cell #1 | 195.3 mAh | 195.5 mAh | 195.4 mAh |
| Cell #2 | 193.8 mAh | 194 mAh | 193.9 mAh |
| Cell #3 | 196.4 mAh | 196.5 mAh | 196.45 mAh |
| Cell #4 | 197.1 mAh | 197.2 mAh | 197.15 mAh |
| | | | 195.725 mAh |

**Table. S2** Geometry of the jellyroll and 1D model

| Parameters | Values | Source |
|---|---|---|
| 3D geometry of the jellyroll | | |
| $t^j$ | 5.6 mm | Measured |
| $w^j$ | 18.2 mm | Measured |
| $\delta^c$ | 0.122 mm | Measured |
| $\delta^a$ | 0.247 mm | Measured |
| $\delta^{se}$ | 0.018 mm | Measured |

| | | |
|---|---|---|
| $\delta^{pc}$ | 0.015 mm | Measured |
| $\delta^{nc}$ | 0.012 mm | Measured |
| $H^{j}$ | 30 mm | Measured |
| $L^{j}$ | 265 mm | Measured |
| Geometry of the 1D model | | |
| $L^{ps}$ | $\left(\delta^{c}-\delta^{pc}\right)/2$ | Estimated |
| $L^{ng}$ | $\left(\delta^{a}-\delta^{nc}\right)/2$ | Estimated |
| $L^{se}$ | $\delta^{se}$ | Estimated |
| $S^{j}$ | $2L_{j}H_{j}$ | Estimated |

**Table. S3** The material parameters of the SIBs

| Parameters | Unit | Jellyroll | Ball |
|---|---|---|---|
| Heat capacity | $J/\left(kg\ K\right)$ | $C^{j}=2425.32$ [b] | $C^{ball}=475$ [1] |
| Thermal conductivity | W/(m K) | $k_{a}^{j}=33.84$<br>$k_{r}^{j}=1.7056$ [b] | $k^{ball}=44.5$ [1] |
| Heat transfer coefficient of air | W/(m$^2$ K) | $h^{air}=25$ [b] | |
| Surface emissivity | 1 | $\varepsilon_{Df}=0.9$ [b] | |
| Ambient temperature | °C | $T_{amb}=26.3695$ [c] | |

| Parameters | Unit | Cathode | Separator | Anode | Jellyroll | Ball |
|---|---|---|---|---|---|---|
| Density | $kg/m^3$ | $\rho^{Al}=2770$ <br> $\rho^{c}=2900$ [a] | $\rho^{se}=817.7$ [c] | $\rho^{Al}=2770$ <br> $\rho^{a}=800$ [a] | $\rho^{j}=1212.5$ [c] | $\rho^{ball}=7850$ |
| Elastic constants | $MPa$ | $E^{c}=2275$ [c] | $E^{se}=555$ [c] | $E^{a}=2260$ [c] | $E^{j}=430$ [c] | $E^{ball}=207000$ |
| Poisson' ratio | 1 | $v^{c}=0.3$ | $v^{se}=0.3$ | $v^{a}=0.3$ | $v^{j}=0.3$ | $v^{ball}=0.3$ |
| Strain hardening | / | | $A^{se}=200.31MPa$ <br> $n^{se}=0.518$ [d] | | | |
| Electrical conductivity | S/m | $\kappa^{c}=50$ [2] | $\kappa^{se}=0.7325$ | $\kappa^{a}=256$ [2] | | |
| Diffusion coefficient | $m^2/s$ | $D^{c}\left(c_{\mathrm{NVPF}}\right)$ [2] | $D^{se}=1.81\times10^{-10}$ | $D^{a}\left(c_{\mathrm{HC}}\right)$ [2] | | |
| Maximum concentration | $mol/m^3$ | $c_{eq}^{c}=15148$ [a] | | $c_{eq}^{a}=8357$ [a] | | |
| Equilibrium potential | V | $E_{eq}^{c}\left(c_{\mathrm{NNMF}}\right)$ [3] | | $E_{eq}^{a}\left(c_{\mathrm{HC}}\right)$ [2] | | |
| Rate constant | $m/s$ | $k^{c}\left(c_{\mathrm{NVPF}}\right)$ [2] | | $k^{a}\left(c_{\mathrm{HC}}\right)$ [2] | | |

[a] Directly from manufacturer's data or calculated

$$c_{1,m}^{\max} = 3.6\frac{\rho_m Q_m^{\max}}{F}, \quad m = \{n, p\}$$

$$c_{1,n}^{\max} = 3.6\frac{\rho_n Q_n^{\max}}{F} = 3.6\times\frac{0.8\times10^6\left[g/m^3\right]\times280\left[mAh/g\right]}{96485\left[C/mol\right]} = 8357.78\left[mol/m^3\right]$$

$$c_{1,p}^{\max} = 3.6\frac{\rho_p Q_p^{\max}}{F} = 3.6\times\frac{2.9\times10^6\left[g/m^3\right]\times140\left[mAh/g\right]}{96485\left[C/mol\right]} = 15148.47\left[mol/m^3\right]$$

$$\rho^{cathode} = \frac{\rho^c\left(\delta^c - \delta^{pc}\right) + \rho^{Al}\delta^{pc}}{\delta^c}$$

$$= \frac{2900\left[kg/m^3\right]\times\left(0.122\left[mm\right] - 0.015\left[mm\right]\right) + 2770\left[kg/m^3\right]\times0.015\left[mm\right]}{0.122\left[mm\right]} = 2884.02[kg/m^3]$$

$$\rho^{anode} = \frac{\rho^a\left(\delta^a - \delta^{nc}\right) + \rho^{Al}\delta^{nc}}{\delta^a}$$

$$= \frac{800\left[kg/m^3\right]\times\left(0.247\left[mm\right] - 0.012\left[mm\right]\right) + 2770\left[kg/m^3\right]\times0.012\left[mm\right]}{0.247\left[mm\right]} = 895.71[kg/m^3]$$

[b] Estimated based on ref. [1,4]

[c] Measured

[d] Based on the experimental fit

**Table. S4** The main equations of governing computational framework [4–10]

| 3D mechanical model | |
|---|---|
| Function name | Function |
| Governing equation | $\rho\frac{\partial^2 u}{\partial t^2} = \nabla_X(F_L S) + F_V$ |
| 1D electrochemical model | |
| Solid potential | $i_s = -\sigma_s^{\text{eff}}\nabla\phi_s$ |
| Electrolyte potential | $i_e = -\sigma_e^{\text{eff}}\nabla\phi_e + \frac{2\sigma_e^{\text{eff}}RT}{F}\left(1+\frac{d\ln f}{d\ln c_i}\right)(1-t_+)\nabla\ln c_e$ |
| Transport in solid | $\frac{\partial c_s}{\partial t} = D_s\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_s}{\partial r}\right)$ |

| | |
|---|---|
| Boundary conditions | $\frac{\partial c_s}{\partial r}\|_{r=0} = 0$, $-D_s \frac{\partial c_s}{\partial r}\|_{r=r_s} = \frac{j^{Li}}{a_s F}$ |
| Transport in electrolyte | $\varepsilon_e \frac{\partial c_e}{\partial t} = \nabla \cdot \left(D_e^{\mathrm{eff}} \nabla c_e\right) + \frac{a j_{\mathrm{loc}}}{F}(1 - t_+)$ |
| Reaction rate | $j_{\mathrm{loc}} = j_0 \left\{ \exp\left(\frac{\alpha^{\mathrm{ng}} \eta F}{R_g T}\right) - \exp\left(\frac{-\alpha^{\mathrm{ps}} \eta F}{R_g T}\right) \right\}$ |
| Overpotential | $\eta = \phi_s - \phi_e - U$ |
| Initial condition | $c_e = c_e^0$, $c_s = c_s^0$, $T = T^0$ |
| 3D Thermal model | |
| Governing equation | $\rho C_p \left(\frac{\partial T}{\partial t} + u \Delta T\right) + \nabla \cdot \mathbf{q} = Q \quad \mathbf{q} = -k \nabla T$ |
| Total heat | $Q_s = Q_{cell} + Q_{ISC}$ |
| Total heat dissipation | $q_{loss} = q_{conv} + q_{rad}$ |
| Convection | $q_{conv} = h(T_{amb} - T)$ |
| Radiation | $q_{rad} = \varepsilon_{Df} \sigma_{B-D} (T_{amb}^4 - T^4)$ |
| ISC model | |
| ISC current | $I_{ISC} = \frac{E_{Cell}}{R_{ISC} + R_{Cell}}$ |
| ISC heat | $Q_{ISC} = I_{ISC}{}^2 R_{ISC} \varphi$ |
| Battery heat | $Q_{Cell} = I_{ISC}^2 \cdot R_{Cell}$ |
| ISC resistance | $R_{ISC} = R_0 (1 - \varepsilon_z)$ |

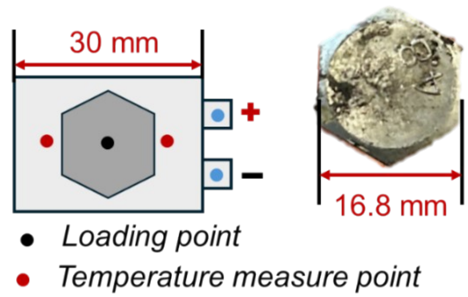


**Fig. S1** Schematic of indenter position and K-type thermocouple placement for ball indentation testing

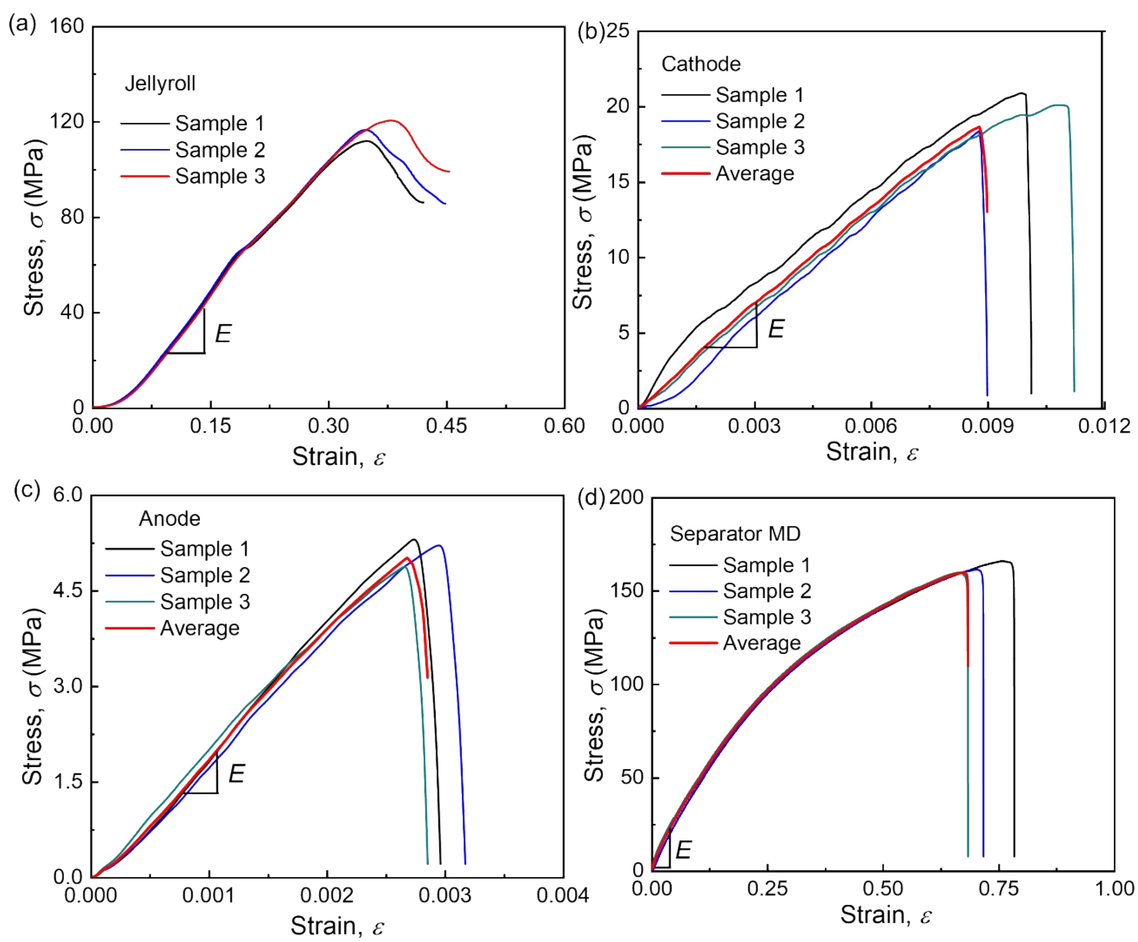


**Fig. S2** Stress-strain curve for (a) the compression test of jellyroll (b) the tensile test of cathode (c) the tensile test of anode (d) the tensile test of separator (machine direction).

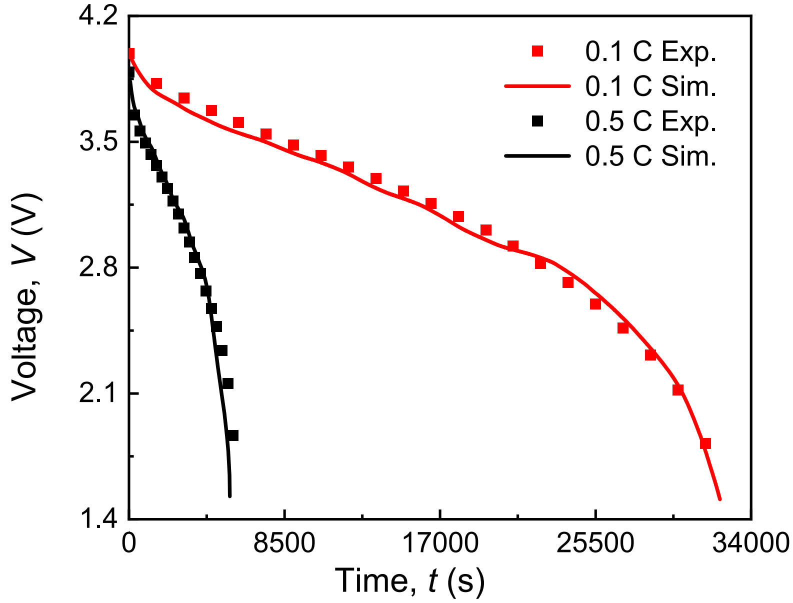


**Fig. S3** The experiment data and computation data of discharge voltage-time curve

## Supplementary Videos

**Video 1.** Ball indentation test of sodium-ion pouch cell at 100% SOC.

## References


1 B. Liu, S. Yin and J. Xu, *Appl. Energy*, 2016, **183**, 278–289.
2 K. Chayambuka, G. Mulder, D. L. Danilov and P. H. L. Notten, *Electrochim. Acta*, 2022, **404**, 139764.
3 D. Kim, E. Lee, M. Slater, W. Lu, S. Rood and C. S. Johnson, *Electrochem. Commun.*, 2012, **18**, 66–69.
4 H. Li, D. Zhou, M. Zhang, B. Liu and C. Zhang, *Energy*, 2023, **263**, 126027.
5 B. Liu, Y. Jia, J. Li, S. Yin, C. Yuan, Z. Hu, L. Wang, Y. Li and J. Xu, *J. Mater. Chem. A*, 2018, **6**, 21475–21484.
6 X. Feng, X. He, M. Ouyang, L. Wang, L. Lu, D. Ren and S. Santhanagopalan, *J. Electrochem. Soc.*, 2018, **165**, A3748.
7 P. T. Coman, E. C. Darcy, C. T. Veje and R. E. White, *J. Electrochem. Soc.*, 2017, **164**, A587.
8 M. Doyle, J. Newman, A. S. Gozdz, C. N. Schmutz and J.-M. Tarascon, *J. Electrochem. Soc.*, 1996, **143**, 1890.
9 M. Doyle, T. F. Fuller and J. Newman, *J. Electrochem. Soc.*, 1993, **140**, 1526.
10 M. Doyle and J. Newman, *Electrochim. Acta.*, 1995, **40**, 2191–2196.