Composite Structural Battery with Modified Carbon Fiber as Anode

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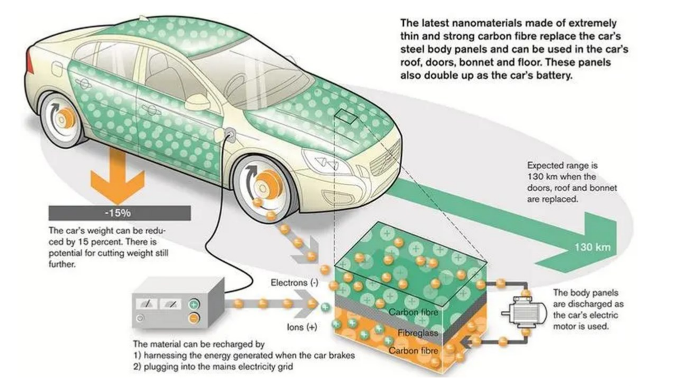
1 Background

- Structural components of future electric and hybrid-electric vehicles featuring energy storage will bring enormous opportunities for weight reduction.
- Composite structural battery is multifunctional fiber-reinforced composites possessing both load bearing and energy storage capabilities, which allows for large mass and volume savings.



Composite structural battery in electric vehicle(EV)

2 Fabrication and characterization

- The modified CFs were synthesized by a four-step method. The SEM showed that the modified layer was uniformly grown on the surface of carbon fiber successfully.

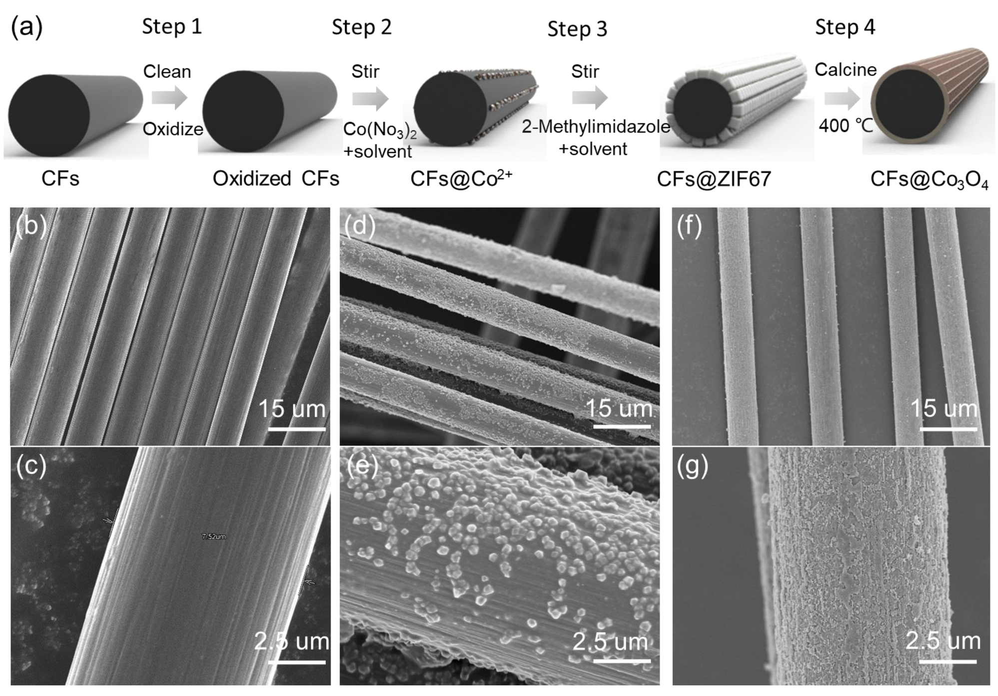


Fig. 1 (a) Schematic of the synthesis of modified CFs; (b–c) SEM images of cleaned and oxidized CFs in 1500 and 9000 times magnification, respectively; (d–e) SEM images of CFs with ZIF67 attached on the surface (CFs@ZIF67) in 1500 and 9000 times magnification, respectively; (f–g) SEM images of CFs with Co3O4 attached on the surface (CFs@Co3O4) in 1500 and 9000 times magnification, respectively.

- Button batteries with modified CFs as anode were fabricated to characterize the electrochemical performance and compared with those unmodified.
- The voltage curves as a function of time were measured by the constant current charge/discharge techniques with a rate of 0.1 C. Batteries based on unmodified and modified CFs exhibited first-cycle gravimetric reversible capacities of 143 mAh/g and 216 mAh/g, respectively.

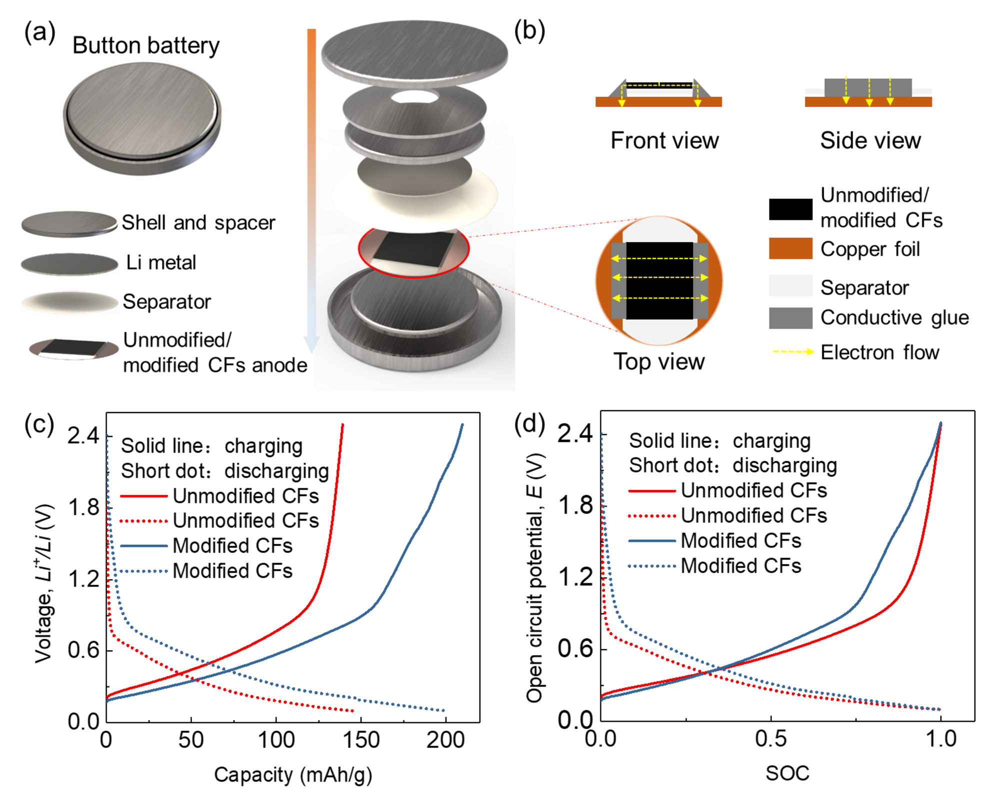


Fig. 2 Fabrication and electrochemical characterization of the button battery. (a) Structural diagram of button battery and (b) unmodified/modified CFs anode; (c) charge and discharge testing for unmodified/modified CFs anode material; and (d) the OCP–SOC curves established by changing the x-axis of (c) to SOC (SOC is equal to current capacity divided by the maximum capacity).

3 Multiphsics modeling and validation

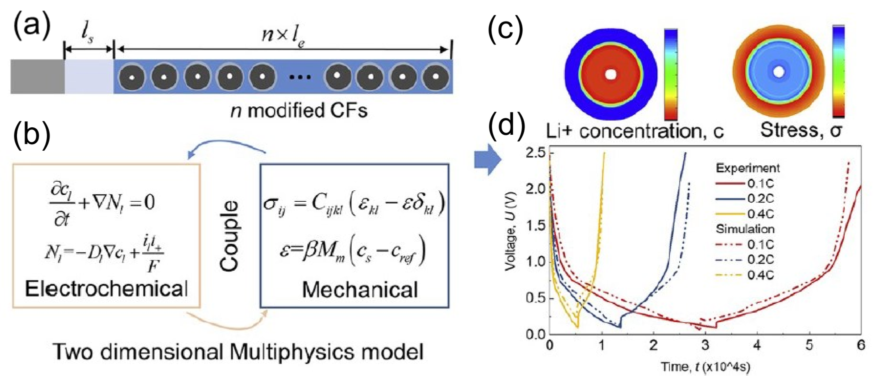


Fig. 3. (a) simplified 2D battery model and RVE of modified CFs anode; (b) coupling strategy of multiphysics model; (c) profiles of radial stress across the radius and contour of radial stress when SOC=1, respectively; (d) model validation in respect to voltage at three different charge/discharge rates.

- A two-dimensional model of a battery using modified carbon fiber as the positive electrode and lithium metal sheet as the negative electrode was constructed.
- Results at three different charge/discharge rates are proved to well predict the voltage-time curves of experimental data within a voltage range of 0.05–2.5 V, which verifies that the accuracy of the 2D multiphysical battery model during charge and discharge.

4 Modeling of modified carbon fiber anode

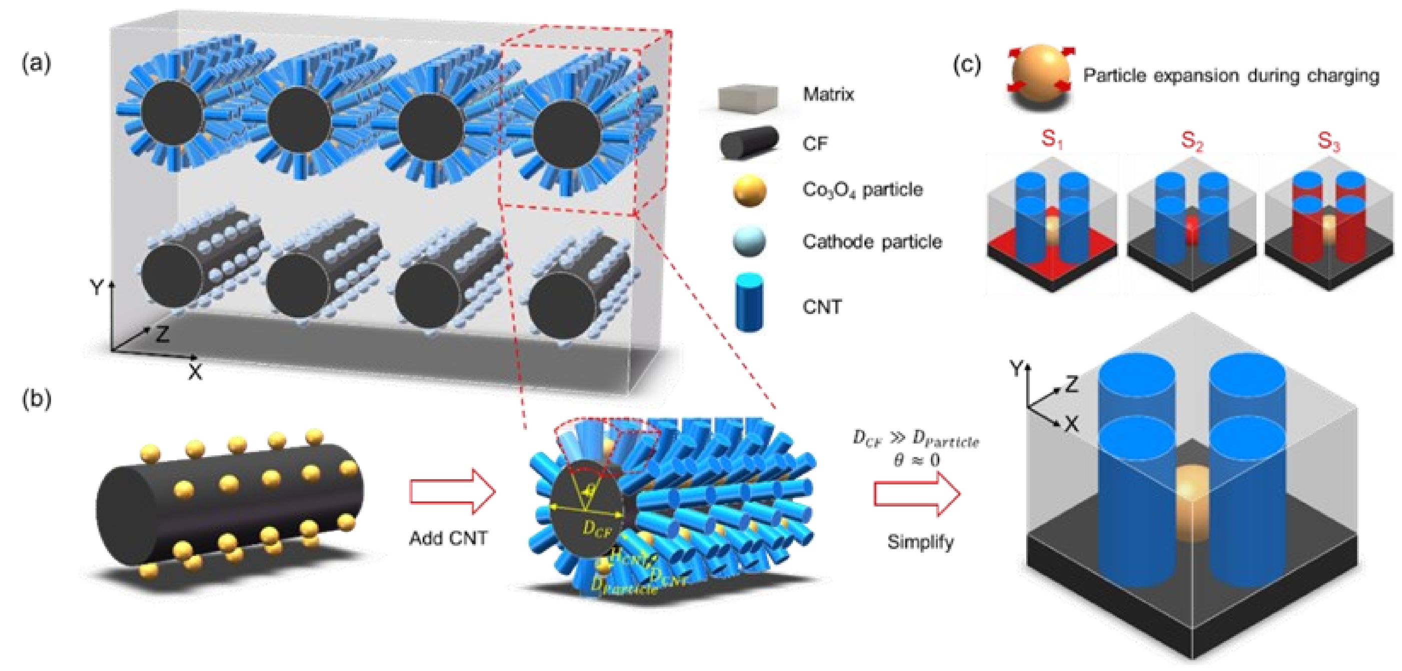


Fig. 4. (a) Schematic of structural battery with Co3O4/CNT modified carbon fiber as anode; (b) simplified model for analysis; (c) three typical interfaces: CF/matrix interface (S1), particle/matrix interface (S2) and CNT/matrix interface (S3).

- The composite structural battery proposed here is composed of a Co3O4/CNT-modified CF anode, a CF-based cathode and a polymer electrolyte.
- The interfacial behavior at three typical interfaces were investigated during electrochemical charging/discharging: CF/matrix interface (S1), particle/matrix interface (S2) and CNT/matrix interface (S3).

5 Interfacial behavior after the addition of CNTs

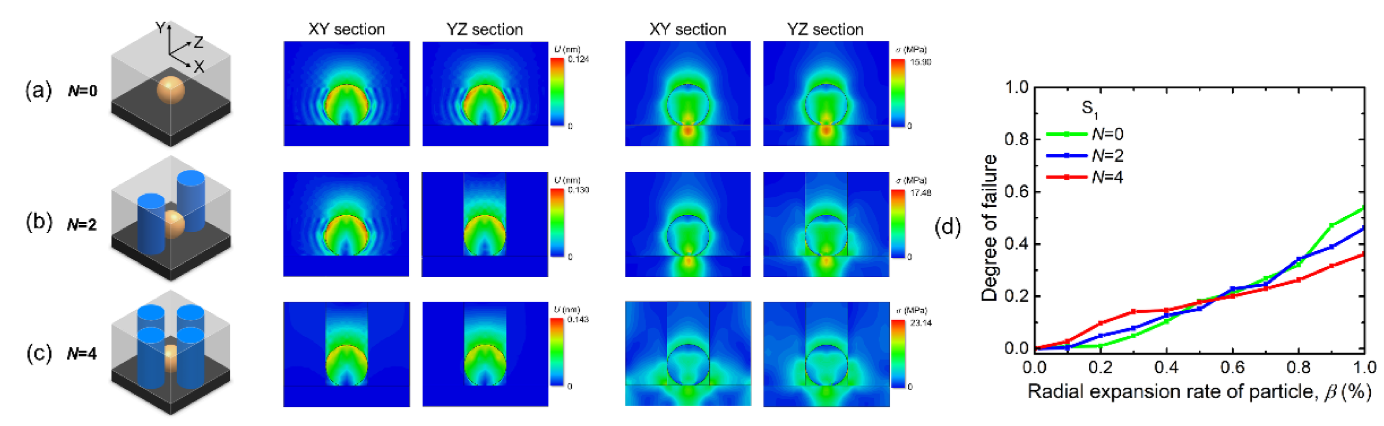


Fig. 5. Comparison of stress and displacement distribution of CF anode with different CNT numbers: (a) N=0, (b) N=2, and (c) N=4; (d) degree of failure at S1 interface with different numbers of CNTs during particle expansion.

- After the addition of CNTs, the deformation of particles was restricted and thus moved toward Y-direction, comparing with the radial deformation without CNTs.
- The overall stress level increased, and the maximum stress appeared at the contact point between particle and CNTs, comparing with that occurred between particle and CF for those without CNTs.

6 Effects of failure parameters

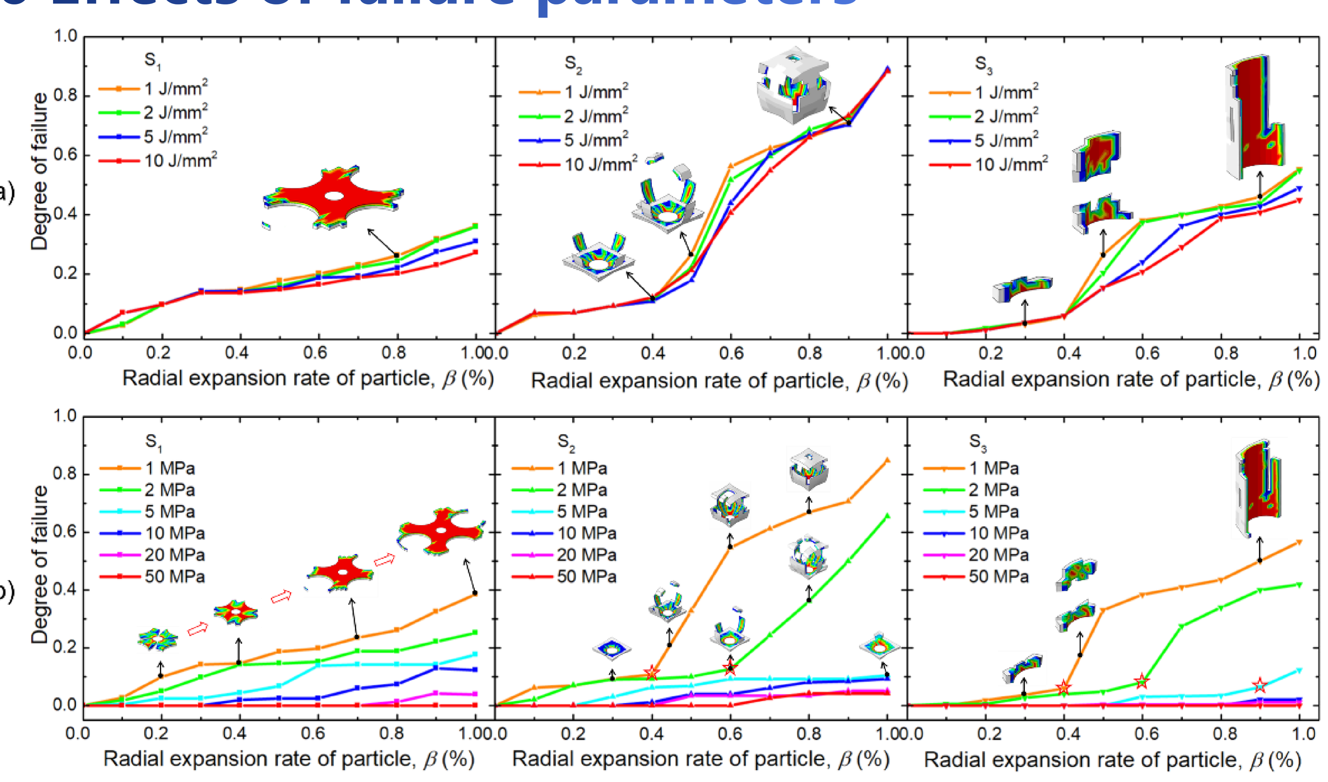


Fig. 6. Degree of failure at each interface during particle expansion with different failure parameters: (a) fracture energy; (b) initial traction.

- Interfacial failure criterion parameters are vital for the corresponding failure mode.
- The degree of failure at different fracture energy does not differ significantly .
- Considering the trade-off between mechanical and electrochemical property of structural electrolytes, 5 MPa is an ideal interfacial strength to achieve better multifunctional performance.

7 Effects of particle patterns

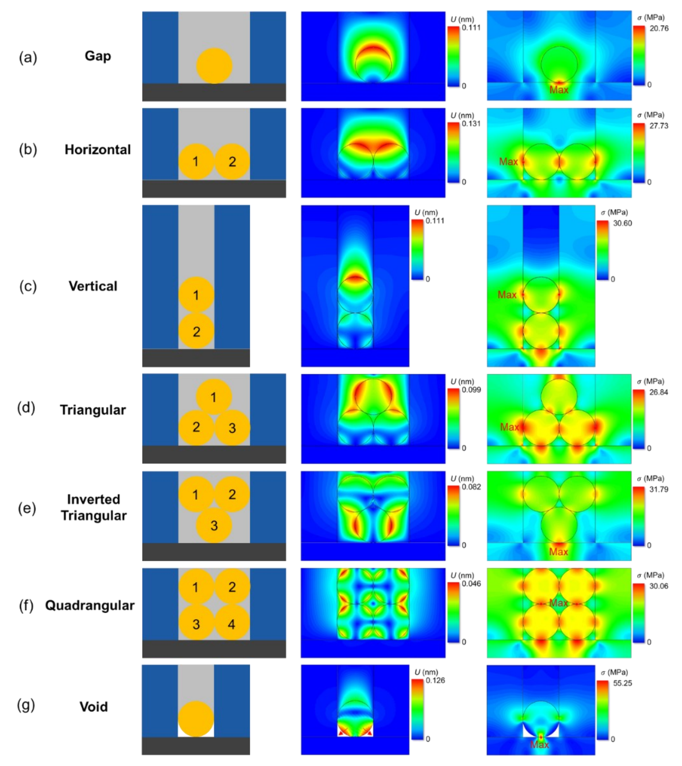


Fig. 7. Comparison of displacement and stress distribution among models with different particle shapes.

- As particle density increased in the quadrangular model, electrochemical failure of active particles happened prior to mechanical failure of composites battery, indicated by the earlier failure at interface S2 than S1 and S3.
- Unlike horizontal and original models, failure at interface S1 in the vertical model was delayed.
- The voids could absorb particle deformation, and the interfacial stress at S3 decreased.

8 Conclusion

- Multifunctional composites served as structural battery show promising prospects. Modified CFs with greater capacity as the structural electrode was fabricated and studied through an electrochemical-mechanical coupled numerical model.
- The simulation method is of great significance to study the electrochemical, mechanical and interfacial performance of composite structural battery. It also provides guides and insights for fabrication of structural battery.
- The interfacial failure behavior as electrochemical charging/discharging was investigated by simulation. The findings provide novel pathways for the design and fabrication of composite structural batteries with high interfacial stability. For example, particle patterns with non-uniform density to decrease stress level near CF interface and enable sufficient deformation outward would be the best.