A02-0383 - *(Digital Presentation)* Accelerating the Conversion Process of Polysulfides in High Mass Loading Sulfur Cathode for the Longevity Li-S Battery

Wednesday, 1 June 2022

13:30 - 13:50

Vancouver Convention Center - West Meeting Room 110

Abstract

Conventional lithium-ion batteries are unable to meet the increasing demands for high-energy storage systems, because of their limited theoretical capacity.[1] In recent years, intensive attention has been paid to enhancing battery energy storage capability to satisfy the increasing energy demand in modern society and reduce the average energy capacity cost. Among the candidates for next generation high energy storage systems, the lithium sulfur battery is especially attractive because of its high theoretical specific energy (around 2600 W h kg-1) and potential cost reduction. In addition, sulfur is a cost effective and environmentally friendly material due to its abundance and low-toxicity. [2]

Despite all of these advantages, the practical application of lithium sulfur batteries to date has been hindered by a series of obstacles, including low active material loading, poor cycle life, and sluggish sulfur conversion kinetics.[3]

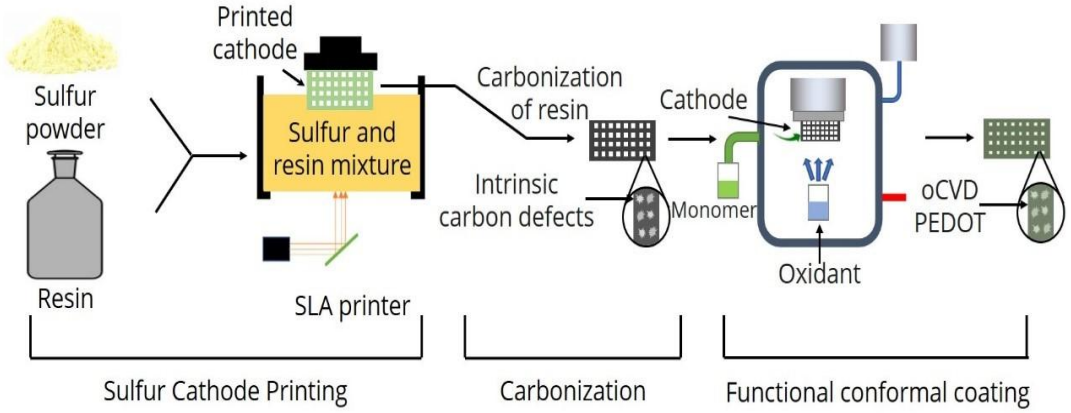
Achieving high mass loading cathode in the traditional 2D planar thick electrode has been challenged. The high distorsion of the traditional planar thick electrodes for ion/electron transfer leads to the limited utilization of active materials and high resistance, which eventually results in restricted energy density and accelerated electrode failure.[4] Furthermore, of the electrolyte to pores in the cathode and utilization ratio of active materials. Catalysts such as MnO_2 and Co dopants were employed to accelerate the sulfur conversion reaction during the charge and discharge process.[5] However, catalysts based on transition metals suffer from poor electronic conductivity. Other catalysts such as transition metal dopants are also limited due to the increased process complexities. . In addition, the severe shuttle effects in Li-S batteries may lead to fast failures of the battery. Constructing a protection layer on the separator for limiting the transmission of soluble polysulfides is considered an effective way to eliminate the shuttle phenomenon. However, the soluble sulfides still can largely dissolve around the cathode side causing the sluggish reaction condition for sulfur conversion.[5]

To mitigate the issues above, herein we demonstrate a novel sulfur electrode design strategy enabled by additive manufacturing and oxidative vapor deposition (oCVD). Specifically, the electrode is strategically designed into a hierarchal hollow structure via stereolithography technique to increase sulfur usage. The active material concentration loaded to the battery cathode is controlled precisely during 3D printing by adjusting the

number of printed layers. Owing to its freedom in geometry and structure, the suggested design is expected to improve the Li ions and electron transport rate considerably, and hence, the battery power density. The printed cathode is sintered at 700 °C at N_2 atmosphere to achieve carbonization of the cathode during which intrinsic carbon defects (e.g., pentagon carbon) as catalytic defect sites are in-situ generated on the cathode. The intrinsic carbon defects equipped with adequate electronic conductivity. The sintered 3D cathode is then transferred to the oCVD chamber for depositing a thin PEDOT layer as a protection layer to restrict dissolutions of sulfur compounds in the cathode. Density functional theory calculation reveals the electronic state variance between the structures with and without defects, the structure with defects demonstrates the higher kinetic condition for sulfur conversion. To further identify the favorable reaction dynamic process, the in-situ XRD is used to characterize the transformation between soluble and insoluble polysulfides, which is the main barrier in the charge and discharge process of Li-S batteries. The results show the oCVD coated 3D printed sulfur cathode exhibits a much higher kinetic process for sulfur conversion, which benefits from the highly tailored hierarchal hollow structure and the defects engineering on the cathode. Further, the oCVD coated 3D printed sulfur cathode also demonstrates higher stability during long cycling enabled by the oCVD PEDOT protection layer, which is verified by an absorption energy calculation of polysulfides at PEDOT. Such modeling and analysis help to elucidate the fundamental mechanisms that govern cathode performance and degradation in Li-S batteries. The current study also provides design strategies for the sulfur cathode as well as selection approaches to novel battery systems.

References:

1. Bhargav, A., (2020). Lithium-Sulfur Batteries: Attaining the Critical Metrics. Joule *4*, 285-291.
2. Chung, S.-H., (2018). Progress on the Critical Parameters for Lithium–Sulfur Batteries to be Practically Viable. Advanced Functional Materials *28*, 1801188.
3. Peng, H.-J.,(2017). Review on High-Loading and High-Energy Lithium–Sulfur Batteries. Advanced Energy Materials *7*, 1700260.
4. Chu, T., (2021). 3D printing-enabled advanced electrode architecture design. Carbon Energy *3*, 424-439.
5. Shi, Z., (2021). Defect Engineering for Expediting Li–S Chemistry: Strategies, Mechanisms, and Perspectives. Advanced Energy Materials *11*.



Presenting Authors

Yuxuan Zhang
Purdue University

Authors

K

Thomas Kivevele

Nelson Mandela African Institution of Science and Technology

S

Han Wook Song

Korea Research Institute of Standard and Science (KRISS)

Corresponding Author

L

Sunghwan Lee

Purdue University

ECS Meeting 241st Li-S.pdf Download

0:00 / 14:53

Ask a question or comment on this session (not intended for technical support questions).

Have a question or comment? Enter it here.

View Related