Electrochemical energy storage performance analysis of carbon based porous materials based on high temperature decomposition

Jialong Song¹*, Mingfen Sun¹

¹Zhuhai College of Jilin University, Zhuhai, Guangdong, 519041, China

*E-mail: sjl@jluzh.edu.cn

Abstract. Carbon based porous materials have low energy storage capacity, poor utilization rate and poor electrochemical storage performance. Therefore, this paper proposes an analytical method for electrochemical energy storage performance of carbon based porous materials based on high temperature decomposition. By analyzing the structure of carbon based porous materials, the parameters affecting the properties of low-carbon porous materials were obtained. The chemical properties of carbon based porous materials were studied. The carbon based porous materials were modified by high-temperature decomposition method to improve the power storage capacity of carbon based porous materials. The experimental results show that the high temperature decomposition of carbon based porous materials has strong energy storage performance, which can effectively improve the energy storage capacity of carbon based porous materials.

1. Introduction

At present, the research on carbon carbon porous materials mainly focuses on increasing specific surface area and introducing multi-stage pore structure[1]. However, due to the accumulation of carbon based porous materials, resulting in smaller specific surface area, the energy storage mechanism of carbon based porous materials exists in the form of electric double layer capacitance, so it is difficult to be widely applied. It is the main method to solve the problem of low capacitance by introducing Eagle capacitor energy storage into the conventional electrochemical energy storage performance analysis method of carbon based porous materials[2-3]. In the aspect of structure design, manufacturing multi-dimensional composite carbon based porous materials can effectively improve their electrochemical energy storage performance. On this basis, an analytical method of electrochemical energy storage performance of carbon based porous materials based on high temperature decomposition is proposed. The method has good chemical stability and low cost due to its high power density and charge discharge efficiency.

2. Electrochemical analysis of porous carbon based energy storage materials

2.1 structure analysis of carbon based porous materials

They combine carbon based porous materials with spherical structures organically to form regular geometry, good fluidity, adjustable porosity and controllable size distribution⁴,⁵. Based on this, the common structures of carbon nanospheres are shown as follows:
In these structures, carbon nanospheres are widely used in catalysis, adsorption, water or air purification, energy storage and conversion. In recent years, a large number of studies have been carried out on the synthesis, characterization and application of carbon nanospheres in carbon based porous materials\cite{6}. Carbon nanospheres are advanced carbon based porous materials with high dispersion, controllable size and pore size, adjustable specific surface area, diverse surface characteristics and ordered structure. The overall performance parameters of carbon porous materials are further standardized, as shown in the table below:

| Material                  | Energy density (wh/kg) | Power density (w/kg) | Charge and discharge times |
|---------------------------|------------------------|----------------------|---------------------------|
| Traditional capacitor    | 0.1-0.2                | $10^6$               | >50                       |
| Supercapacitor           | 0.2-20                 | $1*10^5$             | >100                      |
| Rechargeable battery     | 20-200                 | $<500$               | >50                       |
| Lithium sulfur battery   | 200-400                | $\leq 1500$          | >100                      |

The electrochemical energy storage was studied by carbon adsorption and carbon based porous materials covering. This method is mainly used to optimize pore structure, increase sulfur load, absorb polysulfide, inhibit polysulfide leakage and improve battery performance. In the aspect of pore capacity, the introduction of sulfur is conducive to sulfur absorption, but the adsorption of polysulfide is poor due to the large pore size, which will directly affect the sulfur content of the sample, and make the battery can not work normally. Sulfur content directly affects the capacity of lithium batteries.

### 2.2 Study on chemical properties of carbon based porous materials

Carbon based porous materials have good electrical conductivity, large specific surface area but small specific volume; when carbon porous materials are combined with metal oxides or conductive polymers, the conductivity is higher, which is conducive to the rapid transfer of charge in the redox reaction.

When the scanning speed is 200 mV/s, the specific capacitance of 14 UF/cm² can still be achieved, and the specific capacitance can still be maintained after 5000 cycles. Assuming the acquisition nodes $A_1$, $A_2$ and $A_3$, the formula is as follows:

$$M = \sum_{i=1}^{x} 14 * M_i (A_i - A_2 - A_3) \ (1)$$

$$R = \sum_{i=1}^{x} 200 R_i / (M - M_i)^2 \ (2)$$
In the formula, $M_i$ and $R_i$ are the values of different nodes. Distributed processing can improve the matching rate of chemical structure data retrieval. The electrolyte includes polymer matrix, plasticizer and other polymer matrix supporting battery separator. The electrolyte has good performance, power density and stability. The main properties are shown in the table below.

### Table 2 basic properties of electrolytes

| Polymerization structure | element | temperature | Melting temperature |
|--------------------------|---------|-------------|---------------------|
| PEO                     | -(CH₂CH₂O)$_n$ | -62         | 65                  |
| PAN                      | -(CH₂CH₂(CN))$_n$ | 134        | 314                 |
| Polymethyl methacrylate  | -(CH₂CH₂(CN₃))$_n$ | 104         | 160                 |
| PMMA                     | -(CH₂CHCL)$_n$ | 75          | 210                 |
| PVC                      | -(CH₂CF₂)$_n$ | 60          | 172                 |
| PVDF                     | -(CH₂CF₂)$_n$ | 80          | 134                 |
| HFP                      | -(CH₂CF₂)(CF₂CF(CF₃))$_m$ | -65        | 241                 |

2.3 Electrochemical energy storage algorithm for carbon based porous materials
The existence of layered porous structure is the premise to ensure the rapid transfer of materials, electrolytes and ions. Therefore, the existence of layered porous structure is the key. The preparation of porous carbon based materials by vapor deposition is one of the common methods. However, carbon deposition is usually non selective. Carbon deposits exist on the channels and surfaces of zeolites, which block the internal channels and surfaces of zeolites, restrict the diffusion of carbon sources in the channels, and make the prepared carbon based porous materials uneven. Therefore, the two carbon phase equivalent algorithm is used to optimize and obtain the overall stable flow value.

$$
P_C = \begin{cases} 
\frac{P_A^2 - P_L}{1 + P_A \sum_{i=1}^n \left( \frac{c/R}{\alpha_p^2} \right)^2} + P_A, & P_A \geq P_L \\
0, & P_A < P_L 
\end{cases} (3)
$$

Among the above variables, $P_C$ represents the overall stable flow value, $P_A$ represents the external control ampere flow value, $P_L$ represents the conventional flow value, $R$ represents the average resistance value, $\alpha_p$ is the crude oil leakage coefficient, $c$ is the abnormal gain flow value. When the value of the abnormal gain amplifier is changed, the amplifier will also change. On the whole, the activated carbon hollow spheres prepared by us have good electrochemical performance in acidic and alkaline electrolyte, and have strong adaptability. Other parameter algorithms are as follows:

$$
\lambda = 6P_C f(A) (4)
$$

$$
\varsigma = a - \text{hess}6 / R^a_{2^{n+1}} f(A) (5)
$$

$$
\begin{align*}
B_{2^{n+1}}^n f(A) &= \sum_{j=1}^n B(s-2n)B_{2^n}^n f(A) \\
C_{2^{n+1}}^n f(A) &= \sum_{j=1}^n B(s-2n)C_{2^n}^n f(A)
\end{align*} (6)
$$

In the calculation of chemical energy storage performance in carbon based porous materials, $S$ is the energy storage probability, $\lambda$ is the stable working coefficient, and $B$ is the internal capacity. Based on the simulation energy consumption and impurity purity, the following formula is derived
\[ f'(A) = B_{2^{j=1}}^{n} f(A) + \sum_{j=1}^{n-1} w_j C_{2^{j-1}}^{n} f(A) = \sum_{j=1}^{n} C \lambda + \sum_{j=1}^{n-1} B \zeta \] (7)

Through the above algorithm, the difference of electric energy collected on the electrochemical energy storage surface of carbon based porous materials can be calculated effectively. The electrochemical energy storage of carbon based porous materials is heterogeneous. The detailed regions are extracted and compared, and the accurate analysis of detail regions is realized by using different feature marks and recognition methods.

3. Analysis of experimental results
In order to verify the analysis effect of electrochemical energy storage performance of carbon based porous materials, simulation experiments were carried out. For the powder sample, the battery pack test electrode was prepared by slurry coating process; the weighed materials, conductive carbon black (conductive agent) and polyvinylidene fluoride adhesive were crushed and mixed in a grinding basin, put into a weighing bottle, add an appropriate amount of 1-methyl 1-2-benzopyrrolidone (NMP), and stir with a mechanical stirrer for 4-5 h, and the slurry is uniform. Then, the slurry is evenly coated on the aluminum sheet with a diameter of 12 mm, and then it is put into the oven, and the vacuum drying temperature is 600 °C. In other words, 10 MPa tablet press was used to compact and dry the electrode sheet, and the weight of the electrode sheet was weighed, and the mass of the active substance was calculated according to the mass of the electrode piece before and after.

Table 3 experimental parameter setting

| Experimental apparatus                  | Specifications   | Manufacturer                           |
|----------------------------------------|------------------|----------------------------------------|
| Chemical workstation                   | CHI620E          | Shanghai Chenhua Instrument Co., Ltd   |
| Electronic balance                     | FA2204B          | Shanghai Jinghai company               |
| scanning electron microscope           | HITACHI S-4800   | Japan Co., Ltd                         |
| Projection electron microscope         | HITACHI H-7650   | Japan Co., Ltd                         |
| Numerical control ultrasonic cleaner   | KQ-100DA         | Beijing Deke                           |
| Ultraviolet visible spectrophotometer  | UV-2450          | Tianjin Guangfu Technology             |
| Low speed centrifuge                   | LD4-2            | Beijing Medical Centrifuge factory     |
| Digital constant current power supply  | WLS              | Hangzhou meizan Electronic Co., Ltd    |
| PH meter                               | PHS-3CT          | Chongqing OUYU Technology              |

Based on the above experimental environment, the analysis results of the traditional method and the method in this paper are compared. In order to ensure the research effect, the experimental steps are standardized as follows:

1. The sample was activated with hydrogen oxygen K, and the ratio of hexachloro hydrogen oxygen K to HC was 1:6. First disperse hexachloroethane in water, add Koh, then add a small amount of water, stir and dry. The sample was heated to 600 °C / min in nitrogen atmosphere, then calcined to 600 °C / min, and then stored for 1.5 hours. The activated hollow activated spheres, named A-Hc, were prepared by acid washing, water washing and drying.

2. SEM scanning (scanning SEM, hitach-4800): the samples were dispersed in ethanol and ultrasonic, dropped into water 5 min after silicon wafer, and dried. When testing, it is necessary to inject gold powder and then sample at different speed.

Tecanig2f20s-tw: the samples were dispersed in ethanol solution and ultrasonic solution with 5 ms ultrasonic wave, dropped on copper wire, and dried. Samples at various rates.

3. EDX and feteiercan2f20s twtw: used for the analysis of carbon, C, N and elements in mappi samples.

4. X-ray photoelectron spectroscopy: paste the sample on the transparent tape and test its full spectrum.
5. X-ray diffraction (XRD, x'pert-prompd, diffractometer: sample scanning to 900)

6. 50 mg sample was collected according to Brunauer Emmett tell e and microporous adsorption equipment, and nitrogen adsorption was separated according to microporous model.

7. Thermogravimetric analysis: nitrogen atmosphere 10-C / mi 8000 °C / min M.

Based on the above experimental steps, the performance analysis results of the two methods are compared, as shown in the following figure:

![Fig. 3 structure analysis and comparison of porous materials](image)

According to the figure, the storage capacity of different methods is different. When the time is 0.1min, the storage capacity of traditional method 1 is 632 W, that of traditional method 2 is 186w, and that of this method is 840w. When the time increases to 0.5 min, the storage capacity of traditional method 1 is 705W, that of traditional method 2 is 412w, and that of this method is 1100W. The results show that the modified carbon based porous materials have good electrochemical energy storage performance.

4. Conclusion

Carbon based porous carbon materials have become the carrier of active sulfur in sulfur-containing batteries because of their porous, light-weight and good conductivity. However, it has been found that the inhibition of sulfide shuttle effect by porous carbon based materials is still limited. The heterogenous element atom is replaced by the original carbon atom, and the polysulfide in the electrolyte is chemisorption and adsorption, which limits its retention in the positive electrode area, and improves the cycle life and capacity of the positive electrode. In order to further improve the sulfur storage performance of carbon based porous materials, the enhanced adsorption of metal compounds on the surface of carbon based materials or metal composite materials is usually needed to
further improve the sulfur cathode performance. The results lay a foundation for the modification of carbon based porous materials by nano metal carbides.

Acknowledgments
This work was supported by Guangdong Province Key Platforms and Major Research Projects(No. 2018KQNCX347): Preparation and Modification Positive Materials (NCM523) of Lithium-ion Battery and Electrochemical Properties Study, Innovative Ability Training Project: Preparation and application of silicon / carbon anode materials for lithium ion batteries (2018XJCQ067), and the Quality engineering projects of Zhuhai College of Jilin University: Guangdong Yutian Bali Technology Co., Ltd. practice teaching base (ZLGC20190306).

Reference
[1] Xu F, Yan H, Chen J, et al. Ultrafine LiNi1/3Co1/3Mn1/3O2 powders via an enhanced thermal decomposition solid state reaction[J]. Journal of Applied Electrochemistry, 2019, 49(7):647-656.
[2] Zhao H, Afriyie L O, Larm N E, et al. Glycol-functionalized ionic liquids for high-temperature enzymatic ring-opening polymerization[J]. RSC Advances, 2018, 8(63):36025-36033.
[3] Hu X C, Wang W W, Jin Z, et al. Transition metal nanoparticles supported La-promoted MgO as catalysts for hydrogen production via catalytic decomposition of ammonia[J]. Journal of Energy Chemistry, 2019, 38(5):41-49.
[4] Tarantino S C, Zema M, Callegari A M, et al. Monoclinic-to-orthorhombic phase transition in Cu2(AsO4) (OH) olivenite at high temperature: strain and mode decomposition analyses[J]. Mineralogical Magazine, 2018, 82(2):347-365.
[5] Veerababu R, Satya P K, Karamched P S, et al. Austenite stability and M2C carbide decomposition in experimental secondary hardening ultra-high strength steels during high temperature austenitizing treatments[J]. Materials Characterization, 2018, 144(4):191-204.
[6] Permin D A, Gavrishchuk E M, Kut'In A M, et al. Simultaneous Thermal Analysis of Reactions Underlying Self-Propagating High-Temperature Synthesis of Scandium Oxide Powders[J]. Inorganic Materials, 2019, 55(2):149-154.