Polymer Composites in Energy Based on Fluid Mechanics

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Abstract: As a kind of clean energy, thermoelectric material has attracted great attention. It can realize the conversion between heat energy to electric energy, and electric energy to heat energy. In recent years, conductive polymer materials have been widely used in thermoelectric materials due to their rich resources, easy processing and synthesis, and especially their low thermal conductivity. This paper aims to study the application of hydro-based polymer composites in energy. This paper begins with a brief introduction to the polymer composite, using the ADINA numerical computing platform for partial polymer composites. Treat the liquefied soil as a non-Newtonian fluid, using the analysis method of flow-solid coupling. According to the basic theory of flow-solid coupling, first, by establishing a numerical model of lifiable polymer composites, this work focuses on the preparation of Fe and Co and FeCo miscellaneous 2D porous materials. The results of the prepared material by nitrogen absorption and detachment test showed that the material has a good mesoporous structure, high specific surface area (316-372 m²/g). Electrochemical testing of the rotating disk electrode has proved that the oxygen-reduction (ORR) catalytic activity of the material is greatly improved compared to the non-mesoporous metal-to-nitrogen-doped carbon material. It is proved that the actual preparation value of the polymer composite and the simulated preparation value are wrong, and the minimum difference of NWD is only 0.05104. The preparation is basically stable, while the mixed polymer composite material can effectively control its specific capacitance value, to prepare a better and more stable polymer composite material.

1. Introduction

With the expansion of social production scale, the improvement of people's living standards and the increasing number of car ownership, the consumption of non-renewable fossil fuels such as coal, oil and natural gas is increasing, and the natural gas produced by fossil fuels uses a large amount of greenhouse gases. Gases such as NOX and SOX also have strong effects on the natural environment. The International Energy Agency predicts that by 2035, fossil fuels will account for 82% of the world's energy sources. As China's oil resources are being exhausted, global oil reserves will
decline, and oil prices will rise, casting a shadow over economic growth and industrial development.

In the polymer composites based on fluid mechanics in the application of energy research, a lot of scholars to study, and achieve good results, such as: Nuermaimaiti W and others found through the theoretical calculation of the polymer nanofiber thermoelectric optimal value can reach about 15, which also shows that the polymer materials have great potential in the field of thermoelectric [3]. Al Lafi A G led a team to find for the first time that iodine-doped polyethylene polymer materials showed macroscopic electrical properties. This major experimental discovery became a turning point of traditional ideas, leading people to the belief that insulated polymer materials can become conductive materials, and inspiring people to start the extensive exploration and research of [4] in the structure and electrical properties of polymer materials.

This paper begins with a brief introduction to the polymer composite, Using the ADINA numerical computing platform for partial polymer composites, Treat the liquefied soil as a non-Newtonian fluid, Using the analysis method of flow-solid coupling, According to the basic theory of flow-solid coupling, First, by establishing a numerical model of lifiable polymer composites, This work focuses on the preparation of Fe and Co and FeCo miscellaneous 2 D porous materials, The results of the prepared material by nitrogen absorption and detachment test showed that, The material has a good mesoporous structure, High specific surface area (316-372 m² / g), Electrochemical testing of the rotating disk electrode has proved that the oxygen-reduction (ORR) catalytic activity of the material is greatly improved compared to the non-mesoporous metal-to-nitrogen-doped carbon material.

2. Research on Hydro-Based Polymer Composites in Energy

2.1 Conductive Isotropic Polymer Composite Material

Conductive isotropic polymer composite is usually referred to as conductive polymer composite. In the first stage of the development of conductive polymer composite materials, the polymer matrix used is mostly monophasic polymer, but this kind of conductive polymer composite materials to achieve the requirements of conductive performance, usually need to add a lot of conductive filler, so invisible cause composite system melt viscosity increase, so the system has greater processing difficulty and high penetration threshold, and the cost is greatly increased. After a lot of theoretical research, the researchers try to introduce conductive particles into duplex or heterogeneous incompatible blend system, to achieve the purpose to overcome the above defects, the results found that composite penetration threshold has obvious downward trend, and on the basis of the put forward the "double overpenetration" conductive mechanism, namely conductive particles in incompatible blend phase, and the continuous phase and in another phase. Since then, the conductive polymer composites with incompatible mixture as the matrix has attracted unprecedented wide attention. At the same time, in different series of conductive fillers, the conductive polymer composite material with carbon black as the conductive fillers is also the most concerned composite conductive materials in the composite conductive polymer materials. Therefore, this paper mainly makes a simple introduction of the related discussion of polymer conductive composites, [5-6].

2.2 Electrochemical Performance Test

The working electrode was manufactured as follows by grinding the active material, carbon
black, and PVC, mixed with ethanol at a mass ratio of 80:10:10. The resulting slurry was applied to
the treated nickel foam substrate (1cm 1cm) and then dried at 80°C for 24 hours and pressed before
testing. Among them, the CV test is between 0–0.7V s (relative to SCE), at different scan rates. The
GCD is measured at the potential range of 0–0.45V (relative to SCE) at different current densities;
the EIS test is conducted at an open circuit voltage, at 10-2105Hz, and at an AC amplitude of 5mV.
The cycle performance of the prepared samples was determined by the LAND test system to obtain
[7-8] after 2,000 charge and discharge cycles in the potential range of 0–0.45V and at the current
density of 5Ag-1.

2.3 Algorithm Selection

This paper describes the working principle of water-based rechargeable Zn-PANTHI batteries.
During the charging process of the rechargeable battery, the Zn2 + in the electrolyte is reduced and
deposited on the outside of the Zn electrode, while the copolymer is oxidized. In contrast, when the
discharge process occurs, the precipitated Zn is oxidized to Zn2 + and released into the electrolyte,
while the copolymer is reduced. The results of the charge-discharge reaction process have many
similarities with the previously mentioned reports of Zn-poly (aniline-Tianqing B) cells and
Zn-poly (aniline-N-methionine) cells. Considering the overall structure of the PANTHI and the
charge-discharge mechanism of the polyaniline, the electrode reaction of the Zn-PANTHI
copolymer cell is as shown as follows, [9-10]:

negative pole:

\[ \text{PANTHI}^{\text{reduced}} + 2\times \text{CI}^- \rightarrow 2\text{xe}^- \Leftrightarrow \text{PANTHI}^{(2x+1)}(\text{CI}^-)^{2x} \text{X} \left( \text{oxidized} \right) \]  

(1)

positive pole:

\[ x\text{Zn}^{2+} + 2\text{xe}^- \Leftrightarrow x\text{Z} \]  

(2)

2.4 Construction of Polymer Energy Model Based on Fluid Dynamics

During a turbulent reaction, the reaction dynamics and the turbulent mixing process can affect
both the chemical reaction process, especially for parallel competition reactions, which has a great
impact on the selectivity of the reaction. When the turbulent mixing mass is very good, the reaction
is completely controlled by the dynamics; when the turbulent mixing mass is extremely poor, the
reaction is completely controlled by the mixing. The finite rate / vortex dissipation model is
proposed based on this case, considering the influence of two factors on the reaction process.

Chemical reaction process must occur through molecular contact, and fluid mechanics is based
on the grid solution, the simulation of less than the grid scale process is inaccurate, requiring the
corresponding method, namely the micro mixing model, to describe the small scale mixing and
chemical reaction process. Thus, the standard coil suction model [11-12] describing the microscopic
mixing process is introduced based on the finite rate / vortex dissipation model.

2.5 Comparison of the Thermal Stability of the Electrode Materials
The results of the thermal stability tests for PANI, TCN, and PANI / TCN 8-2 are shown in Figure 1. Because the moisture in the sample cannot be completely removed, all the tested materials have a certain mass loss at around 100 °C. Mass loss of 10% of the TCN upon heating from 100 °C to 600 °C, likely due to the decomposition of the TCN surface by unreduced oxygen-containing functional groups. The mass loss of PANI is up to 54% due to the decomposition of the structure at high temperature. The weight curves of PANI / TCN 8-2 is between PANI and TCN. The mass loss between 100 °C and 200 °C is small, while heating from 200 °C to 600 °C causes a accelerated 17% loss of the entire material mass due to the decomposition of the PANI structure in the composite. The above study results show that the thermal stability of PANI when modified with a small amount of TCN was greatly improved.

3. Research and design of polymer composite posites in energy

3.1 Preparation of Working Electrodes

Ni-MOF powder (80wt%), polyvinylidene difluoride (PVDF, 10wt%) and acetylene black (10wt%) and a small amount of anhydrous ethanol were ground in a mortar to form a slurry and applied to NF to obtain the Ni-MOF powder electrode. The prepared electrodes were dried in a 70°C blast drying tank overnight, after which one end of the coated Ni-MOF powder was flattened with 10 MPa pressure, resulting in a load mass of the Ni-MOF powder of approximately 1.8 mg cm^-2. The AC electrode was prepared in the same way as the Ni-MOF powder electrode.
3.2 Experimental Design

This paper for the energy model of polymer composite test, is the first of the preparation of polymer composite experiment, due to technical reasons and other reasons, the actual value of the material prepared and simulated value have a big difference, so this paper selected three polymer composite material, the production comparison, the difference between the actual value and the simulated value. The second is to explore the specific capacitor value of polymer composite materials, to explore the specific capacitor value of two different polymer materials and its mixed polymer materials, and to analyze the more excellent polymer materials.

4. Experimental Analysis of the Application of Polymer Composites in Energy

4.1 Comparison of Simulated Values and Actual Values

Due to production environmental factors and production industrial factors, the actual manufacturing and simulated preparation values of polymer composite materials are somewhat different. In this paper, the design experiment and three common polymer composites are selected for preparation to record the difference between the simulated value and the actual production value. The experimental data are shown in Table 1.

<table>
<thead>
<tr>
<th></th>
<th>NWD</th>
<th>MWD</th>
<th>PDI</th>
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<tr>
<td>analog value</td>
<td>1.72×10⁴</td>
<td>5.9×10⁴</td>
<td>3.43×10⁴</td>
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<tr>
<td>actual value</td>
<td>1.68×10⁴</td>
<td>8.98×10⁴</td>
<td>5.36×10⁴</td>
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</table>

Table 1. Differences between the simulated preparation values of the polymeric composites and the actual preparation system

Figure 2. Actual preparation of three different polymer composites
As can be seen from Figure 2, compared to the simulation preparation, the actual preparation is only lower than the simulation preparation value due to the existence of technical and environmental factors, but in contrast, the actual preparation of NWD material is the most similar to the simulation preparation, with the difference of only 0.0510^4 Can better ensure the stability of the actual production value.

### 4.2 Specific Capacitance Value

In this paper, the energy application of composite polymerization materials is mainly for the study of their capacitance. By comparing separate polymerization materials and the difference between the proportional 1:1 mixed materials, the comparison of more suitable materials for energy applications is explored.

**Table 2. Differences between the specific capacitance values of the two separate polymerized materials and their mixing**

<table>
<thead>
<tr>
<th></th>
<th>0</th>
<th>2</th>
<th>4</th>
<th>6</th>
<th>8</th>
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<tr>
<td>TCN</td>
<td>130</td>
<td>90</td>
<td>80</td>
<td>80</td>
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<tr>
<td>PANI</td>
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<td>240</td>
<td>230</td>
<td>220</td>
<td>210</td>
<td>200</td>
</tr>
<tr>
<td>PANI/TCN5-5</td>
<td>245</td>
<td>210</td>
<td>170</td>
<td>165</td>
<td>160</td>
<td>160</td>
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</table>

**Figure 3. Comparison of the specific capacitance values of the three different polymers**
As can be seen from FIG. 3, the specific capacitance value varies greatly between the different materials, and the specific capacitance value of the mixture is located between the two specific capacitance values. With the concentration, the higher side approaches. Therefore, how to reasonably control the concentration to produce a polymer composite material with relatively high and stable specific capacitor value is the future research direction.

5. Conclusions

In this paper, different polymers are selected as couplers to adjust oxide distribution, connect graphene and oxides, and protect oxide particles, and several different composites are designed for different metal oxides and corresponding applications to realize the controllable growth of metal oxides on the surface of graphene. The protection of metal oxides or metal particles is realized by coating or hybridization. In this paper, PPy / EG composite was prepared by in situ polymerization, and the conductivity of PPy / EG composite was increased significantly, and the power factor was greatly increased. The micromorphology and structure of the prepared electrode materials were studied and analyzed by a series of characterization methods. At the same time, CV, GCD and EIS electrochemical test methods were used to test the electrochemical properties of materials in energy storage devices. Conductive polymers have the advantages of light weight, good electrical conductivity, good mechanical flexibility, low cost, and affordable economy, so it is a promising development direction to apply the conductive polymer layer to the conformal substrate of flexible electronics and energy devices. For energy storage device electrode materials, most of the existing conductive polymer electrodes are combined with carbon materials to improve the stability and electrical conductivity.

References


