Finite-Element Analysis on Percolation Performance of Foam Zinc

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ABSTRACT: With the aid of X-ray microcomputed tomography and digital image processing technology, the three-dimensional structure of foam zinc prepared by the electrodeposition process is reconstructed. Furthermore, a simplified finite-element model of foam zinc, which can more accurately reflect its structure, is proposed. Based on the Brinkman—Forchheimer-extended-Darcy law, the finite-element method is used for the numerical simulation of the percolation performance of the foam zinc. The results indicate that for high-porosity foam zinc, the pore density is the main factor affecting its percolation performance. A function is established to describe the relationship between the pore density and pressure drop. To obtain an optimum structure, a tetrakaidecahedron cylinder model is established and compared to a previously built model, and the comparison demonstrates that the optimized model performs better in the field of percolation performance.

1. INTRODUCTION

The rechargeable metal—air battery has advantages such as low cost, environmental friendliness, and high safety performance; especially, zinc—air batteries are expected to be one of the most promising new energy batteries for the next generation because of their high energy density.1–4 The theoretical energy density can reach as high as 1350 kW h kg−1.5–7 However, because of technical limitations, the rechargeable zinc—air batteries have not yet been commercialized.8–10 Taking the zinc anode as an example, it is much denser and has a smaller specific surface area; dendritic or mossy growth of zinc results in the morphology and shape change during the charging/discharging process, leading to the decline in the performance and the low cycling stability of the battery.11,12

Because of its three-dimensional (3D) through-pore structure, foam metal has a low density, high specific surface area, low flow resistance, good mechanical properties, and good thermal management performance.13,14 As a structural and functional integrated material,15,16 foam metal can be used as an electrode material for batteries. Foam Zn electrode with a higher specific surface area increases the charge/discharge capacity and enhances the rated performance of batteries; therefore, the charge/discharge efficiency of the battery is improved and the energy loss is reduced. The pores can also provide sufficient space for the growth of dendrites formed by the Zn electrode during the charging/discharging process, improving the performance of the Zn electrode and providing the flow channel of the electrolyte. The good performance of the foamed structure on the thermal management can improve the heat dissipation efficiency and the thermal failure of materials or structures resulting from the heat concentration during the battery charging and discharging process.17 The high porosity of the porous structure can greatly reduce the density of the electrode, reducing the weight of the battery to increase the current density per unit mass, and promoting the development of low-weight and heterotrophic battery cells. The researchers studied the percolation properties of foam metal with gas and liquid as working fluids.18,19 It was found that the increase in pressure drop is exponentially related to pore density.19 For foam metals with a high porosity, a large number of irregular zigzag flow channels can continuously disturb the fluid boundary layer.20 Fluid flow often occurs as reflux, turbulence, and unsteady flow, making the influencing factors of seepage characteristics extremely complex.21,22,23 The performance analysis of porous materials has been carried out using simplified mathematical models.24,25 Although these models are quite different from the actual structure of foam metal, they are relatively simple and easy to be used for experimental analysis, and the simulation results are consistent with most experimental results.26,27 The applications of the finite-element method in numerical simulation of the percolation properties of foam metal is of great practical significance.28,29 Studies on percolation properties of foam zinc contribute to comprehend the flow behavior of electrolyte in foam zinc electrode, which could provide a theoretical basis for the selection of the pore structure parameters of foam zinc as the anode of the zinc—air battery regarding the flow resistance.

At first, foam zinc as the research object in this study is prepared by the ultrasonic-assisted electrodeposition process.30 The 3D structure of the foam zinc is reconstructed. Furthermore, a simplified finite-element model of the foam zinc, which can reflect its actual structure, is proposed. Based on the Brinkman—Forchheimer-extended-Darcy law, the finite-element method13,32 is applied in the finite-element analysis.
(FEA) for revealing the quantitative relationship between the pore structure and the percolation performance of foam zinc, and the foam zinc structure is optimized. Through the numerical simulation of the related process, a continuous and complete performance curve of the pressure drop and flow velocity is obtained,23,33 which provides the theoretical basis for the selection of the pore structure parameters of foam zinc as the anode of the zinc−air battery and shortens the test period.

2. RESULTS AND DISCUSSION

The average pore diameter $d_p$ of the foam zinc samples obtained by the electrodeposition process is measured using the direct section observation method. Based on this, foam zinc cell models with different parameters were established. According to the pore density, it can be divided into four types: 10, 25, 45, and 70 PPI and 90, 93, 95, and 97%, respectively, according to porosity. The pore structure parameters are presented in Table 1. There are about 700 000 nodes and 340 000 elements in the tetrakaidecahedron triprism cell model.

| $d_p$ (mm) | pore density (PPI) | porosity (%) |
|------------|-------------------|--------------|
| 5.35       | 10                | 90           |
| 5.35       | 10                | 93           |
| 5.35       | 10                | 95           |
| 5.35       | 10                | 97           |
| 2.16       | 25                | 97           |
| 1.14       | 45                | 97           |
| 0.67       | 70                | 97           |

2.1. Validation of FEA. The finite-element model of foam zinc with a pore density of 10 PPI and porosity of 93% is selected, and the pressure drop of foam zinc per unit length at different velocities is calculated; the results of the comparison are presented in Figure 1. Figure 1 presents the FEA results compared to the experimental results using water as the fluid.

By comparison, it is found that the FEA results agree well with the experimental results and the data available in the literature.17,24 It is revealed that the model and finite-element method established in this paper can be applied to the research on the percolation performance of foam metal.

2.2. Influence of Porosity on the Percolation Performance of Foam Zinc. Foam zinc samples with a pore density of 10 PPI and porosity varying from 90 to 97% are selected as the objects to study the influence of porosity on the percolation properties of foam metal. A part of the FEA is presented in Figure 2. Figure 2 indicates that with the flow rate $v$ increasing from 0.4 to 1.2 m s$^{-1}$, the unit pressure drop $\Delta P/L$ increases continuously, and the growth rate of the unit pressure drop $\Delta P/L$ increases with the flow rate $v$. Under the same flow rate, the unit pressure drop $\Delta P/L$ increases continuously with the decrease in porosity. The results indicate that it will lead to an increase in the fluid flow resistance with the increase in flow velocity $v$ or decrease in porosity. It is known from the curve that the unit pressure drop $\Delta P/L$ does not conform to a linear relationship with the flow velocity $v$, indicating that the flow state of the water in the foam zinc with a pore density of 10 PPI and porosity of 90−97% deviates from the laminar state described by Darcy’s law (5).

The pressure difference of unit length $\Delta P/L$ under different velocities $v$ was calculated, and the relationship between these two parameters is illustrated in Figure 3.
The FEA results obtained in Figure 3 are processed to obtain the relationship curve between $\Delta P/Lv$ and the velocity $v$, as shown in Figure 4. The curve indicates that there is a linear relationship between $\Delta P/Lv$ and the flow velocity $v$, that is to say, the unit distance pressure difference $\Delta P/L$ and velocity $v$ exhibit a quadratic function relation, which is in agreement with the Brinkman–Forchheimer-extended-Darcy law (6), indicating that the flow state of the fluid in foam zinc with a pore density of 10 PPI and porosity of 90–97% is a laminar turbulent complex state. Under this condition, the flow resistance of foam zinc is affected by the laminar flow and turbulent flow of the fluid.

The percolation performance of foam metals can be characterized by the viscosity percolation performance coefficient $k_1$ and the inertial percolation performance coefficient $k_2$. The larger $k_1$ and $k_2$ are, the better the percolation performance of the foam metal. The $k_1$ and $k_2$ of foam zinc with a pore density of 10 PPI and porosity of 90–97% can be calculated by the Brinkman–Forchheimer-extended-Darcy law (6) and the relationship curve between $\Delta P/Lv$ and $v$ in Figure 4.

Table 2 indicates that when the pore density of the foam metal is constant, the skeleton of foam metal becomes thinner with the increase in porosity, the effective cross-sectional area of the flow increases, and the resistance to fluid flow decreases. At the same time, as the skeleton of the foam metal gets disturbed, the disturbance of the foam metal skeleton decreases with the porosity of the foam metal, which is beneficial to the fluid flow in that it improves the percolation performance of foam metal.

2.3. Influence of Pore Density on the Percolation Performance of Foam Zinc. Foam zinc samples with a porosity of 97% and pore density varying from 10 to 70 PPI are selected as the objects to study the influence of the pore density on the percolation properties of foam metal. A part of the FEA is shown in Figure 5.

Figure 4. Dependence of $\Delta P/Lv$ on $v$ for foam zinc with a pore density of 10 PPI.

Table 2. Viscosity Percolation Performance Coefficient $k_1$ and Inertial Percolation Performance Coefficient $k_2$ of Foamed Zinc with Different Porosities

| Porosity | $k_1 \times 10^5$ (m²) | $k_2 \times 10^5$ (m) |
|----------|------------------------|---------------------|
| 10 PPI, $\varepsilon = 90$ | 1.87 | 2.13 |
| 10 PPI, $\varepsilon = 93$ | 2.21 | 3.08 |
| 10 PPI, $\varepsilon = 95$ | 2.39 | 4.32 |
| 10 PPI, $\varepsilon = 97$ | 2.94 | 6.77 |

Figure 5. Press distributions of foam zinc with a pore density of 10 PPI and different porosities at flow velocity $v = 0.8$ m s$^{-1}$ ((a) 25 PPI, $\varepsilon = 97$; (b) 70 PPI, $\varepsilon = 97$).

Table 3 indicates that as the pore density of foam zinc increases from 10 to 70 PPI, $k_1$ decreases from $29.40 \times 10^{-8}$ to $0.66 \times 10^{-8}$ m² and $k_2$ decreases from $6.77 \times 10^{-3}$ to $0.84 \times 10^{-3}$ m, which reveals that although the porosity of foam zinc is constant, the low pore density will result in a lower fluid resistance and better percolation performance. Comparing the

Table 3. Viscosity Percolation Performance Coefficient $k_1$ and Inertial Percolation Performance Coefficient $k_2$ of Foamed Zinc with Different Porosities

| Porosity | $k_1 \times 10^5$ (m²) | $k_2 \times 10^5$ (m) |
|----------|------------------------|---------------------|
| 10 PPI, $\varepsilon = 90$ | 29.40 | 6.77 |
| 10 PPI, $\varepsilon = 93$ | 5.09 | 2.90 |
| 10 PPI, $\varepsilon = 95$ | 1.73 | 1.51 |
| 10 PPI, $\varepsilon = 97$ | 0.66 | 0.84 |
ranges of \( k_1 \) and \( k_2 \) in Table 2 with those in Table 1, it is known that under high-porosity (greater than 90%) conditions, the pore density is the main variable that affects the percolation performance.

The Ergun model is an empirical equation based on the pore structure to describe the flow resistance of porous materials. The Ergun-like model has been proposed for foam metals by Dukhan and others.\(^{34-36}\)

\[
\frac{\Delta P}{L} = \frac{1}{7.45 \times 10^7} \left( \frac{1}{d_p} \right) \mu v + \frac{1}{7.72 \times 10^2} \left( \frac{1}{d_p} \right) \rho v^2
\]

(1)

Based on the Ergun-like model, the influence of aperture (pore density) on the percolation performance is investigated in this study. Formula 1 can be written as

\[
\frac{\Delta P}{L} = \frac{1}{d_p} \left( \frac{1}{\varepsilon} \right)^m \mu v + \left( \frac{1}{\varepsilon} \right)^n \left( \frac{1}{d_p} \right)^2 \mu v^2
\]

(2)

\( k_1 \) and \( k_2 \) can be obtained by combining with formula 13

\[
K_1 = \frac{1}{A} d_p^m
\]

(3)

\[
K_2 = \frac{1}{B} d_p^n
\]

(4)

The relationships between \( k_1 \), \( k_2 \), and the aperture \( d_p \) can be obtained from the fitting formulas 3 and 4 with the data of both \( d_p \) in Table 3 and \( k_1 \) and \( k_2 \) in Table 2

\[
K_1 = \frac{1}{7.45 \times 10^7} \left( \frac{1}{d_p} \right) \mu v
\]

(5)

\[
K_2 = \frac{1}{7.72 \times 10^2} \left( \frac{1}{d_p} \right) \rho v^2
\]

(6)

The formula of the flow resistance of the foam zinc with a porosity of 97% is obtained by substituting formulas 5 and 6 into the Forchheimer-extended-Darcy law expression 13

\[
\frac{\Delta P}{L} = \frac{1}{7.45 \times 10^7} \left( \frac{1}{d_p} \right) \mu v + \frac{1}{7.72 \times 10^2} \left( \frac{1}{d_p} \right) \rho v^2
\]

(7)

\((0.67 \text{ mm} \leq d_p \leq 5.35 \text{ mm}, 0.4 \text{ m s}^{-1} \leq v \leq 1.2 \text{ m s}^{-1})\)

3. OPTIMUM STRUCTURAL DESIGN OF FOAM ZINC

The framework of the FEA model, namely, the tetrakaidecahedron tri-prism model of foam zinc based on the real structure, was optimized. A tetrakaidecahedron cylinder model of foam zinc is established, as shown in Figure 7.

The two models with the same pore structure parameters (pore density of 10 PPI and porosity of 97%) are selected for FEA calculation. The definitions of the boundary condition and application of the load are identical. The FEA results of the two different models are presented in Figures 8 and 9.

Figures 8 and 9 indicate that with the increase in flow velocity \( v \), the unit pressure drop \( \Delta P/L \) of the two structures both increases. When the flow velocity \( v \) is constant, the \( \Delta P/L \) of the tetrakaidecahedron cylinder model is smaller, that is to say, it has a lower flow resistance. The \( \Delta P/Lv \) of the two models has a linear relationship with the flow velocity \( v \). The percolation factors of the two models are obtained using a linear fitting method and presented in Table 4.

Table 4 indicates that the tetrakaidecahedron cylinder model has a smaller viscous seepage coefficient and a lower flow resistance but a greater inertial percolation performance coefficient. When the flow velocity \( v \) is increased to a certain extent, the inertial effect gradually replaces the viscous effect as...
optimized 3D network structure can provide theoretical guidance for the preparation of high-performance foam zinc.

In the process of building up the finite-element models and setting the boundary conditions, a reasonable degree of simplification is made in both mathematics and physics. Although the mathematical and physical simplifications are carried out in this article, the conclusions obtained are instructive on predicting the percolation properties of foam zinc.

5. EXPERIMENTAL SECTION

5.1. Experimental Materials. Polyurethane sponge of 10 PPI is used as the matrix, and foam zinc is prepared by the electrodeposition process. The polyurethane foam is cut into the specimen with a size of 140 mm × 110 mm × 15 mm. The specimen is pretreated through the following steps: degreasing, roughening, sensitizing by SnCl4 and PdCl2, and activating and then peptizing before plating. Chemical zinc-plating technology with the assistance of ultrasound is adopted to perform the conductivity treatment. The plating solution is developed according to the formula of Table 5 and then put into the ultrasonic generator. When the ultrasonic power is adjusted to 300 W and the current is adjusted to 12 A, the specimen is immersed in the plating solution. After undergoing electrodeposition for 10 h, the specimen is taken out, washed by clear water, and finally dried in an oven. The foam zinc is processed into the specimen with a size of 60 mm × 40 mm × 10 mm using the wire electrode cutting technology. Foam zinc is heat treated at 360 °C with hydrogen atmosphere for 8 h, and then heat treated at 100–150 °C with hydrogen atmosphere for 8 h to remove polyurethane sponge. Table 5 lists the components of the electroplating solution.

5.2. Calculation Method of Percolation Performance. Assuming the fluid is turbulent in foam zinc without a phase transition, the two-equation $k$–$\varepsilon$ turbulence model is used as follows

$$\frac{dk}{dt} = \frac{\partial k}{\partial t} + \frac{\partial (\tau_{ij} \frac{\partial k}{\partial x_j})}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ -
abla \cdot \left( k \nabla \left( \frac{\varepsilon}{\kappa} \right) \right) \right] + G - \varepsilon $$

$$\frac{d\varepsilon}{dt} = \frac{\partial \varepsilon}{\partial t} + \frac{\partial (\tau_{ij} \frac{\partial \varepsilon}{\partial x_j})}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ -
abla \cdot \left( \varepsilon \nabla \left( \frac{k}{\varepsilon} \right) \right) \right] + (\epsilon G - c_1 \varepsilon) \frac{\varepsilon}{k} $$

where

$$G = \nu \left( \frac{\partial \tau_{ij}}{\partial x_j} \right) \left( \frac{\partial \tau_{ij}}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \right) $$

and

$$\nu = \frac{k}{\varepsilon} $$

Table 4. Viscosity Percolation Performance Coefficient $k_1$ and Inertial Percolation Performance Coefficient $k_2$ of Different Models

| tetrakaidecahedron tri-prism model | tetrakaidecahedron cylinder model |
|-----------------------------------|----------------------------------|
| $k_1 \times 10^7$ (m$^{-1}$)       | 2.94                             |
| $k_2 \times 10^7$ (m$^{-1}$)       | 6.77                             |

Table 5. Components of Electroplating Solution

| component                  | concentration ratio |
|----------------------------|---------------------|
| ZnSO$_4$·7H$_2$O (AR)      | 12–23 g L$^{-1}$    |
| EDTA·2Na (AR)              | 15–20 g L$^{-1}$    |
| HCHO (36%) (AR)           | 10–15 mL L$^{-1}$   |
| KNaC$_4$H$_4$O$_6$·4H$_2$O (AR) | relative          |
| $K_3$Fe(CN)$_6$ (AR)       | relative            |

In this study, we have prepared the open-cell foam zinc by the ultrasonic-assisted electrodeposition process. The tetrakaidecahedron tri-prism model is established based on the real structure using X-ray micro-CT as the FEA model of foam zinc. Furthermore, FEA calculations of the percolation performance of foam zinc are carried out, which indicated that pore density is the main factor affecting the percolation performance of foam zinc. According to the FEA results, the empirical relationship between the fluid flow resistance in foam zinc and the aperture is obtained.

Formula 7 can provide a theoretical basis for the selection of the pore structure parameters of foam zinc as the anode of the zinc–air battery regarding the flow resistance.

The tetrakaidecahedron cylinder model of foam zinc is established by optimizing the tetrakaidecahedron tri-prism model. By comparing the percolation performance of the two models, it can be concluded that the tetrakaidecahedron cylinder model will perform well regarding percolation.
The pressure gradient of $\Delta P / L$ of the fluid in the porous media is linear with velocity $\bar{v}$ under a low flow velocity

$$\frac{\Delta P}{L} = \frac{\mu}{k_1} \bar{v}$$ (12)

The viscous percolation performance coefficient $k_1$ of the foam metal can be calculated using formula 12.

When the flow rate rises, the relationship in the porous media between the pressure gradient $\Delta P / L$ and velocity $\bar{v}$ deviates from the Darcy’s law, where the Brinkman–Forchheimer-extended-Darcy law is satisfied

$$\frac{\Delta P}{L} = \frac{\mu}{k_1} \bar{v} + \frac{\rho}{k_2} \bar{v}^2$$ (13)

The inertial percolation performance coefficient $k_2$ of foam metal can be calculated using formula 13.

Both $k_1$ and $k_2$ are the intrinsic parameters related to the pore structure characteristics of the foam metal, which do not change with the fluid properties. Therefore, these two parameters can be used to describe the percolation performance of the foam metal.

The device for testing the percolation performance of the foam zinc is illustrated in Figure 10. During the experiment, we first investigate the sealing performance of the test device and then open the cooling cycle system for cleaning and cooling using the cycle of deionized water in the device. By adjusting the flow rate $Q_f$, the pressure difference $\Delta P$ of deionized water flowing through the foam zinc samples with different pore densities is measured at different flow rates $\bar{v}$, and $k_1$ and $k_2$ are calculated using the above-mentioned formulas.

Using the Ansys Fluent software package, the standard two-equation $k-\varepsilon$ turbulence model is selected. The material property of the foam metal is set to foam zinc, the fluid is set to water, and the inlet and outlet of the flow channel are, respectively, set to the speed inlet and the pressure outlet. The pore diameter is used as the length scale in the FEA.

5.3. Finite-Element Model of Foam Zinc. The percolation performance test does not destroy the structure of the foam zinc, and the test specimen is used for the microcomputed tomography (micro-CT) scanning. The foam zinc structure is scanned using a Bruker Micro-CT SKYSCAN 1172 (made in Belgium). The acceleration voltage and current of the X-rays are set to 100 kV and 100 $\mu$A,
respectively. During the experiment, although the increment of the fixed angle is set to 0.7°, we select the appropriate scanning resolution of 12 μm for the pore density of 10 PPI and finally produce a set of two-dimensional (2D) tomography images (Figure 11a) of the foam zinc specimens. Using the extreme point threshold method, the approximate range of the gray threshold is determined within the values ranging from 4 to 20 (Figure 11b). The image segmentation is processed in MATLAB, the statistical data of surface density are calculated, and the porosity of foam zinc with a certain threshold is calculated using the Origin software (shown in Table 6).

The 3D structure of pores in the foam zinc is approximately tetrakaidecahedral, whereas the 2D structures are roughly quadrilateral and hexagonal. The tetrakaidecahedron tri-prism model is proposed by cutting off prisms inside the tetrakaidecahedra by the pretreatment module of the ANSYS software. Considering the geometric characteristics of the tetrakaidecahedron, the spatial topology of the original models is based on the close-packed structure; then, we perform Boolean intersection operation with a cylinder. Finally, a simplified finite-element model of foam zinc is proposed, as shown in Figure 11f. Figure 11g shows the tetrakaidecahedron tri-prism cell model, which can accurately reflect the structure of foam zinc.

Table 6. Porosity of Different Thresholds and Experiments

| threshold value (T) | porosity (%) |
|---------------------|--------------|
| 8                   | 94.313       |
| 10                  | 94.301       |
| 12                  | 94.284       |
| 14                  | 94.265       |
| experimental value  | 94.28        |

Figure 11. Procedure of tetrakaidecahedron tri-prism model establishment ((a) 2D tomography image; (b) grayscale maps; (c) full structures; (d, e) partial structure; (f) tetrakaidecahedron tri-prism cell model; (g) tetrakaidecahedron tri-prism model).

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