Morphological characteristics modeling and fluid simulation of metal fiber sintered felt based on growth model and Monte Carlo method

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ABSTRACT

Fibrous porous material has complex special network structure and porosity feature. Effective digital description of these complex micro structures is a challenge that needs to be solved in engineering fields. Building digital model for active design is the basis of function design and manufacturing optimization of related materials. In this paper, a new digital modeling method that aims at metal fibrous porous material is explored based on the growth model viewpoint and using Monte Carlo method. It means to build a parametric feature model which can map the forming processes of these complex micro structures. This feature model makes advances in geometric authenticity and parameters controllability by introducing porosity, gravity and interference as feature control parameters. By comparing the feature attributes with the reverse scanning reconstruction model and combined with fluid simulation experiments, the efficiency of active design model for describing metal fibrous porous structures is verified.

Keywords: Metal fibrous porous material, microstructure modeling, active deign, growth model, Monte Carlo method

1. INTRODUCTION

In recent years, metal fiber porous materials have played an extremely important role in many fields such as new energy manufacturing, chemical industry, environmental protection materials, aerospace, etc. This material has complex spatial network structures and pore characteristics, which significantly affect the performance of various aspects of the material¹. For a long time, due to the lack of effective three-dimensional fine models to describe such complex structures, the calculation and simulation of their related functional coupling have mostly been based on abstract representation models from macroscopic statistical concepts², or simplified model units³. The traditional design and manufacturing theory based on abstract simplification is difficult to guide its morphology and structure design and process optimization, and the basic research on its related application functions is seriously lagging behind the application of this structure. The research on digital design methods for metal fiber porous materials with complex geometric morphology features is a key issue that urgently needs to be solved in many engineering fields and has certain universal significance.

In the research of porous structure modeling, the use of more refined modeling methods to reflect more realistic microstructure characteristics has received attention from the academic community. The main approach in this regard is to use reverse engineering technology to obtain a three-dimensional fine mesh model by performing CT tomography, image processing, and 3D reconstruction on real metal fiber materials⁴. The goal is to approximate the real physical model to support simulation calculations in related fields. However, this reverse reconstruction model uses a large number of discrete grids to represent the three-dimensional morphology, and due to the lack of effective geometric feature description and parameter control, simulation results are difficult to directly optimize geometric features. Scholars have proposed a model design method based on the random distribution of linear elements⁵, and demonstrated a continuous scale description method from simplified features to fine description based on this method. This research approach has important reference significance for active modeling of fiber porous structures.

In order to solve the problems of lack of geometric realism in abstract simplified models and lack of feature description and control in reverse reconstruction models, this paper proposes a CAD feature modeling method for metal fiber porous structures that meets the requirements of active design based on the perspective of growth models. This method refers to the commonly used cutting and molding processes in the manufacturing of metal fiber porous materials⁶. Based on Monte Carlo thinking, it simulates the forming process of a large number of fiber units under the effects of gravity, pressure, and

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International Conference on Optics, Electronics, and Communication Engineering (OECE 2024), edited by Yang Yue, Proc. of SPIE Vol. 13395, 1339503 · © 2024 SPIE · 0277-786X · Published under a Creative Commons Attribution CC-BY 3.0 License · doi: 10.1117/12.3048696 interference. The overall characteristic properties are close to the real physical model, and the micro geometric characteristics and macro statistical information of individual fiber units can be effectively controlled through parameters.

2. METHODOLOGY

2.1 Active design concept based on feature parameters

Introducing the concept of features in the design of complex microstructures can effectively describe their complex morphology and structural information, that is, effectively digitize the description; By controlling parameters associated with features, the generation of micro morphology can be effectively adjusted and controlled, ultimately supporting the design and optimization of materials, i.e. active design.

2.2 Building of fiber unit and main parameters of the model

By observing the fiber network morphology photos obtained by electron microscopy scanning in Figure 1 and referring to statistical data^{3,4}, it can be concluded that the complex metal fiber network structure has the following characteristics:



Figure 1. SEM image of copper fiber sintered plate with a porosity of 90%³.

Fiber network is a spatially connected porous structure formed by a large number of complex and disordered fibers overlapping at sintering nodes;

The fiber segments between sintering nodes have a shape close to a straight-line segment or a smooth arc, while the original fibers exhibit complex spatial spline curve shapes;

The original fiber length is about 20-30 mm, but the fiber segment length between nodes after sintering is usually not more than 1400 um, mainly 200-600 um;

The fiber diameter is roughly between 20 and 100 um, and the cross-sectional shape is close to circular.

Note that the aspect ratio of fiber segments is approximately between 2 and 10. Setting the aspect ratio of fiber unit bodies to 50 can ensure that the length of fiber unit bodies is sufficient to overlap with each other and form nodes. After comprehensive consideration, the metal fiber unit adopts a solid simulation of a circular ring with a smooth arc axis and a circular end face. Its shape is determined by three parameters: chord length L, arc height H, and end face diameter D (Figure 2). This fiber unit is used as an individual to participate in the overall model construction. The metal fiber network overall model is formed by stacking a certain amount of fiber unit in a given cubic space, as shown in Figure 3.



Figure 2. Schematic diagram of fiber unit body.

The main parameters for constructing a fiber unit model are:

- L: The chord length of the fiber unit, with a default value of 5;
- H: Fiber unit body arc height, default value is 1.25;
- D: Fiber unit diameter, default value is 0.2.

The main parameters for constructing the overall model of the fiber network are:

Box: The side length of a cube box, with a default value of 10;

n: The total number of fiber units stacked inside the cube is related to the porosity of the material. If the porosity is 90%, $n\approx$ 400 can be calculated;

nx: The number of random fiber units generated in each step has a significant impact on the density of the fiber network, with a default value of 400;

tor: The distance tolerance for determining whether the fiber unit interferes is the same as the diameter D of the fiber unit end face by default.

2.3 Dynamic construction method of metal fiber network model

2.3.1 Method for constructing fiber network structure. A relatively simple construction method is to uniformly and randomly arrange fiber element bodies in a certain space, similar to the random distribution of linear elements on the plane described in Reference⁵. But in fact, fiber units cannot "float" in the air without support, nor can they penetrate each other.

According to the growth model theory, a growth model is a model used to simulate the characteristics of the growth process⁷. The most essential characteristic is that growth is related to history, that is, the final group depends on the previous group configuration, which is a non-Markov process. For example, some scholars have used the diffusion limited aggregation (DLA) model to simulate the random walking and bonding behavior of various particles during the sintering process of CBN grinding wheels when studying the microstructure, and analyzed the fractal characteristics of the final aggregation model⁸. In this study, the metal fiber network is regarded as a pure local growth model, and its growth law is the overlap and stacking mode between fibers.



Figure 3. Schematic diagram of fiber network heaping up process.

The self-organizing dynamics of metal fiber networks come from both the gravitational force acting on fiber units and the interference between fiber units, which together form the overlap and stacking of fibers. Figure 3 illustrates the forming process of the fiber network under the influence of gravity and interference: the red fibers fall downward until they "touch" other fibers that have already been stacked on the ground and stop falling. Then, they rotate to a lower center of gravity position and reach a stable state. A large number of fibers fall in sequence and eventually pile up into a three-dimensional network structure. The porosity characteristics of this structure are determined by the cube space size box and the number of fibers n.

In terms of specific implementation, the idea of Monte Carlo method was adopted⁹, and a relatively concise algorithm was used to achieve simulation results similar to the above image description. The main idea is to generate a set of nx random fiber units A {f1, f2, ..., fnx} in each step, exclude those sets B that intersect with existing fibers from these fiber units, and select the one with the lowest center of gravity from the remaining set of random fiber units CAB as the result of this iteration. Step k is denoted as f'k. Finally, after n steps, n fibers are stacked to form the final three-dimensional network model $S=\{f'1, f'2, ..., f'n\}$. In the process of excluding intersecting fibers, a distance tolerance tor was used to adjust the tor, which can change the distance between fibers and reflect interference characteristics.

In fact, in the production of metal fiber sintered board materials, after filling a large number of metal fibers in the mold cavity to form a three-dimensional network, molding is also required to make the material denser and uniform¹⁰. The specific method is to increase the number of random fiber units nx in each step mentioned above to obtain fibers with lower center of gravity, ultimately forming a denser fiber network. The density of the fiber network is an external manifestation of gravity and pressure characteristics, which is influenced by the parameters nx and tor together. The third part of this article will demonstrate the different model shapes and geometric information statistics obtained by changing the parameter nx.

2.3.2 Specific geometric problems. In specific calculations, it is necessary to address the spatial orientation and position

of the fiber unit. Space attitude refers to the expression of fiber units at any angle in space, with a focus on generating the axis arcs of the fiber units.

Since arcs are randomly generated in a given cubic space (denoted as BOX), let the starting point of the arc be S (x1, y1, $z1)\in BOX$, the angle between the chord of the arc P and the XY plane be α , the angle between the projection of P on the XY plane and the x-axis be β , the random number $rnd \in (0,1)$, and pi be the circumference. Then we calculate the coordinates of the endpoint E (x2, y2, z2) of the arc. Let the spin angle of the spatial arc around the chord P be γ . Through three-dimensional coordinate transformation, the coordinates of the midpoint M (x3, y3, z3) of the arc can be calculated using equation (1), as shown in Figure 4.



Figure 4. Spatial attitude of fiber axis arc.

$$(x3=(x1+x2)/2-\text{heigh}*(\cos(\text{angle3})*\sin(\text{angle2})+\sin(\text{angle1})*\sin(\text{angle3})*\cos(\text{angle2}))$$

$$y3=(y1+y2)/2+\text{heigh}*(\cos(\text{angle2})*\cos(\text{angle3})-\sin(\text{angle1})*\sin(\text{angle2})*\sin(\text{angle3}))$$

$$(1)$$

$$z3=(z1+z2)/2+\text{heigh}*\sin(\text{angle3})*\cos(\text{angle1})$$

By obtaining the coordinates of the starting point S, midpoint M, and endpoint E, the function AddArc3Pt (S(), M(), E()) can be called to generate a large number of random spatial arcs. Then, search for the nx random arcs generated in each step, exclude the fibers that intersect with the existing fibers, and determine the spatial position of the fibers by finding the one with the lowest center of gravity in the remaining fiber set. After repeating the above operations n times, n fibers are added to the existing fiber set, forming the final 3D network model.

2.4 Geometric information statistics of the model

The geometric information of a three-dimensional network model mainly includes fiber segment length distribution and fiber orientation distribution.

By using the return value array Array of the function CurveCurveIntersection (mycurve1 (i), mycurve2 (j), tor), a series of data can be obtained. The length Rg1, Rg2, Ry1, Ry2, and other numerical values from the starting point to each intersection point can be obtained from Array(). The length of a fiber with three intermediate nodes can be calculated using equation (2). The fiber orientation can be represented by the angle α between the chord P and the XY plane, as well as the angle β between the projection of P on the XY plane and the X-axis, as shown in Figure 4. α and β can be obtained using equation (3).

$$\begin{cases}
Lenth1 = Rg1 \\
Lenth2 = Ry1 - Rg1 \\
Lenth3 = MIN(Rg2, Ry2)
\end{cases}$$
(2)

$$\begin{cases} \alpha = \arcsin((z2-z1)/L) \\ \beta = \arcsin((y2-y1)/(L^*\cos(\alpha))) \end{cases}$$
(3)

3. MORPHOLOGICAL COMPARISON RESULTS AND DISCUSSION

Using the method described in this article, 400 fibers are stacked in a space of $10 \times 10 \times 10$, with fiber unit volume parameters as described earlier. A three-dimensional network model is obtained as shown in the figure. By comparing and analyzing the morphological features, fiber segment length distribution, and orientation distribution of the 3D model reconstructed through reverse engineering⁴, it is shown that this modeling method can effectively describe the characteristics of the

porous structure of metal fibers (Figures 5-7, the left image is the reverse engineering reconstruction model, and the right image is the active design model built in this paper).



Figure 5. Comparison of 3D model morphology.



Figure 7. Comparison of fiber orientation distribution.

Absolute

of the angle between the fiber and

the horizontal plane

By changing the parameter nx mentioned in Section 2.2 above while maintaining the spatial size and total amount of fibers of the experimental cube unchanged, it is possible to simulate fiber network structures with different densities under different pressure compression conditions. Figures 8(a)-8(c) represent the fiber network models generated when nx=25, nx=100, and nx=400, respectively. It can be seen that from Figures 8(a)-8(c), the fiber network gradually tightens and compacts, reflecting the effect of pressure. The comparison chart of segment length distribution Figure 8(d) shows that as nx increases, the average segment length gradually decreases (1.94->1.62->1.38), and the proportion of shorter segment lengths gradually increases. The fiber orientation comparison graph (e) shows that as nx increases, the angle between the fiber and the horizontal plane gradually decreases, and the number of fibers with a large angle with the horizontal plane rapidly decreases.



Figure 8. Comparison of fiber network morphology data with different densities.

4. FLUID SIMULATION EXPERIMENT AND RESULTS

4.1 Fluid simulation experimental methods and settings

From the two models in Figure 5 near the middle, select areas with similar porosity, and cut $2\times2\times2$ mm cubic space materials for each. After surface trimming, Boolean subtraction, and other processing, two fluid domain cubic models are obtained. The corresponding algorithm of ANSYS FLUENT was applied to mesh the model, as shown in Figure 9. The left image shows the material pore fluid domain scanned in reverse (hereinafter referred to as Model A, with a porosity of 87.7%), and the right image shows the material pore fluid domain of the actively designed model (hereinafter referred to as Model B, with a porosity of 87.1%).



Figure 9. Schematic diagram of mesh division in fluid domain.

Using the ANSYS2020R2 version, it already has the classic CFD software package FLUET built-in. Models, mesh partitioning, scheme selection, and parameter settings are imported in the FLUENT module. This includes an inlet flow rate of 0.5 m/s, a default pressure outlet, an inlet fluid temperature of 260 °C, a wall temperature of 280 °C, a 1:1 mixture of methane and water vapor, a wall material of copper, and an assumed flow pattern of incompressible steady-state laminar flow¹¹.

4.2 Analysis of fluid simulation experiment results

Figure 10 shows the numerical simulation experiment results of Model A, and Figure 11 shows the numerical simulation experiment results of Model B. As mentioned earlier, the porosity of the two models is very similar. Through comparative analysis, it is found that the two models have strong similarities in flow velocity distribution, temperature distribution, and pressure distribution. For example, in the flow velocity distribution of the two models, under a flow velocity of 0.5 m/s at the inlet, the maximum flow velocity in the fluid domain is between 1.3-1.4 m/s, and the minimum value is close to 0. In the temperature distribution, the mixed gas at the inlet of 260 °C is basically heated to 280 degrees Celsius after passing through the fluid domain. In the pressure distribution, most of the pressure in the fluid domain is between 0-3 Pa, and there

is a continuous decreasing trend from the inlet to the outlet. The pressure is higher near the wall and lower in the central region of the fluid, which is consistent with practical experience.

This indicates that the B model, which adopts parameterized active design, can better reflect the fluid transmission performance of actual materials. By adjusting the different parameters of the B model, the dependence on the preparation of corresponding physical models and physical experiments can be significantly reduced, and the properties of different types of metal fiber sintered felt materials can be effectively predicted.



Figure 11. Numerical simulation experiment results of Model B.

5. CONCLUSIONS

This article explores the concept of feature modeling in the field of digital design of complex microstructures. Based on the perspective of growth models, porosity, gravity, and interference are introduced as characteristic control parameters in the study of porous metal fiber structures. Monte Carlo method is used to simulate the stacking and pressing process of fiber network structures. A parameter controllable fiber network model is established using CAD software secondary development technology. As an effective digital description of the porous structure of metal fibers, this model approaches the real physical model in terms of overall feature attributes, and can effectively control the micro geometric features and macro statistical features of individual fiber units through parameters, effectively solving the problems of abstract simplified models lacking geometric authenticity and reverse reconstruction models lacking feature description and control. Finally, the effectiveness of this method was demonstrated through FLUNET fluid simulation analysis, providing innovative ideas for the digital active design of complex metal fiber porous structures.

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