Two-dimensional Phase-field Simulation of Pore Evolution in High Temperature Self-lubrication Composites

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Abstract. The phase field model was established based on the free energy function method to simulate the evolution process of microporous matrix. High temperature self-lubricating microporous matrix was prepared by powder metallurgy method, then its porosity was measured under different pore forming agent ratio and addition amount, in order to verify the phase field model. The results show that the simulation value of porosity by phase field method is basically consistent with the experimental value, and the phase field model can be used to simulate the effect of pore forming agent on the pore evolution process of matrix.

1. Introduction
It is expected to obtain high temperature self-lubricating material by preparing the microporous matrix and infiltrating with proper amount of solid lubricant[1]. The material can realize self-lubricating at high temperature and meet the requirements of high-temperature self-lubricating performance under some special working conditions, and has broad application prospect[2-3].

The pore structure of microporous matrix is affected by raw material ratio and sintering process and other parameters [4]. It takes a lot of manpower and material resources to study the influence of these parameters on pore structure by experimental method. However, the computer simulation of the actual test can save resources and reduce costs while obtaining the test results [5]. So in this paper, the phase field model is established based on the free energy function method and verified by experiments. The program is compiled by combining the initial conditions and boundary conditions to simulate the evolution process of microporous matrix.

2. Phase Field Simulation of Microporous Matrix
With the sintering process, the solid-gas interface with high energy is converted to the solid-solid interface with low energy, and the free energy of the system is reduced. The relative density field $\rho$ is used to distinguish particles and pores. The value of $\rho$ is 1 for particles and 0 for pores. Different particles are distinguished by long-range orientation parameter $\eta_i$. At particle $i$, the value of $\eta_i$ is equal to 1 and the value of $\eta_{(j≠i)}$ is 0[6].

The total free energy of the system is as follows [7]:

$$F = \int \left\{ f_0(\rho(r)\eta_1,\ldots,\eta_p) + \frac{a}{2} \sum_{i=1}^{p} \left[ \nabla \eta_i(r) \right]^2 + \frac{b}{2} \left[ \nabla \rho(r) \right]^2 \right\} d^3r \quad (1)$$

The free energy density function of the system is as follows:
where: $F$ is the total free energy of the system; $f_0$ is the free energy density function; $r$ is the position coordinate; $a$ is the interface energy coefficient of long range orientation field; $b$ is the density field coefficient; $A_1, A_2, A_3, A_4, A_5, A_6$ and $A_7$ are phenomenological coefficients.

The evolution equations of density field and phase field are shown in equations (3) and (4)

\[
\frac{dp}{dt} = \nabla \left[ M \frac{\delta F}{\delta p(r,t)} \right]
\]

\[
\frac{dh_i}{dt} = -L \frac{\delta F}{\delta \eta_i(r,t)}
\]

where: $M$ is the parameter of thermodynamic diffusion coefficient and $L$ is the parameter of interfacial mobility.

The Neumann boundary condition is used for the lattice points on the boundary, that is, the values of the boundary points are assigned to the points outside the boundary. The specific procedures are as follows:

if(i==N-1) {ip=N-1;}  
if(i==0) {im=0;}  
if(j==N-1) {jp=N-1;}  
if(j==0) {jm=0;}  

Matlab language is simple and easy to realize organization visualization, but compared with Visual C++, its calculation speed is slow. In order to improve the calculation speed, this paper uses Visual C++ to solve the control equation.

3. Sample Preparation and Experimental Verification

3.1 Test Materials

The decomposition temperature range of single pore forming agent is limited and it is not easy to form through pores [9-10]. Therefore, in this paper the compound pore forming agent was used to prepare cermet matrix. The main test materials used in this paper are M3/2 high speed steel powder, TiC, Co, Y2O3, graphite powder, Cu3P, TiH2, CaCO3 and Al2O3, C36H70O4Zn. The properties of main test materials are shown in Table 1.

| Composition | Metal | Ceramics | Additional component | Compound pore forming agent |
|-------------|-------|----------|-----------------------|-----------------------------|
| Material    | Density | Granularity |
| M3/2 | 8.3 | 26 |
| TiC | 4.93 | 40 |
| Co | 8.9 | 2.5 |
| Y2O3 | 5.01 | 40 |
| graphite | 2.25 | 0.04 |
| Cu3P | 7.15 | 40 |
| TiH2 | 3.76 | 50 |
| CaCO3 | 2.93 | 45 |
| Al2O3 | 3.94 | 48 |
| C36H70O4Zn | 1.095 | 5-6 |

3.2 Preparation Process

In this paper, M3/2 / TiC cermet materials were prepared by powder metallurgy. The raw material powders which were shown in Table 1 is weighed by electronic balance, and the steel ball is weighed according to the ball material ratio of 4:1. The raw material powder, steel ball and anhydrous ethanol are put into the ball mill, and the anhydrous ethanol is added as the ball milling medium. The rotating
speed of the ball mill is 200 r·min\(^{-1}\), and the milling time is 3 h. The milled powder is dried and sieved in PURUI numerical control constant temperature bath. The sieved powder is put into the metal mould and pressed into the green body with a diameter of φ12 mm×30 mm on the Y41-10A hydraulic press. Then, the microporous matrix was sintered in ZT-70-20Y vertical vacuum hot pressing furnace at a heating rate of 5°C·min\(^{-1}\). The main ignition loss temperature of composite pore forming agent (C\(_{36}\)H\(_{70}\)O\(_4\)Zn 400°C, TiH\(_2\) 650°C, CaCO\(_3\) 800°C) was kept for 20 min and 60 min at sintering temperature. The specific sintering process curve is shown in Figure 1.

![Figure 1. Sintering process curve](image)

4. Test Results and Analysis

4.1 Effect of Compound Pore Forming Agent Ratio on Porosity

![Figure 2. Pore evolution of matrix with different pore forming agents](image)

Figure 2 shows the evolution of micropores in the matrix after adding 6% composite pore forming agent and holding at 1250°C for 60min, and the black part represents the pores. Figure 2 (a)-(f) represents the volume ratio of TiH\(_2\) to CaCO\(_3\), which are 10:90, 20:80, 30:70, 40:60, 50:50, and 60:40,
respectively. Each ratio simulates 10 figures and measures porosity, and takes the average value as the simulation value of porosity.

Figure 3 shows the influence curve of TiH$_2$ and CaCO$_3$ volume ratio on matrix porosity. It can be seen from figure 3 that: The simulation value of micro pore evolution of cermet matrix is closed to the experimental value, which proves that the established phase field model can be used to simulate the effect of composite pore forming agent ratio on porosity.

![Influence curve of volume ratio of TiH$_2$ and CaCO$_3$ on porosity](image)

**Figure 3.** Influence curve of volume ratio of TiH$_2$ and CaCO$_3$ on porosity

4.2 Effect of Compound Pore Forming Agent Content on Pore Structure

Figure 4 shows the pore evolution results of matrix after holding at 1250°C for 60min with TiH$_2$ and CaCO$_3$ volume ratio of 40:60. Figure 4 (a)-(f) shows that the matrix powder is added with 0%, 2%, 4%, 6%, 8%, and 10% composite pore forming agents respectively. Each ratio simulates 10 figures and measures porosity, and takes the average value as the simulation value of porosity. It can be seen from Figure 4 that the porosity of sintered body is small without adding pore forming agent, and with the increase of pore forming agent, the porosity of sintered body increases.

![Pore evolution of matrix with different content of pore forming agent](image)

**Figure 4.** Pore evolution of matrix with different content of pore forming agent
Figure 5 shows the influence curve of pore forming agent addition on matrix porosity. It can be seen from Figure 5 that the simulation value of porosity by phase field method is basically consistent with the experimental value, which proves that the established phase field model can be used to simulate the effect of pore forming agent content on matrix porosity.

Figure 5. Influence curve of pore forming agent addition on matrix porosity

Figure 6 shows the SEM images of matrix pore morphology with different amount of pore forming agent. Figure 6 (a), (b), (c) and (d) represent the SEM images of transverse and longitudinal fracture surface of matrix with 2%, 4%, 6% and 8% of composite pore forming agent respectively. It can be seen from Figure 6: with the increase of pore forming agent, the porosity of matrix increases. When 2% - 4% of the composite pore forming agent is added, the permeability of the pore is low; when the amount of the composite pore forming agent is increased to 6% - 8%, the permeability of the pore is better; when the amount of the composite pore forming agent is increased to 8%, less pores with larger pore size will be produced. The experimental results are consistent with the curve in Figure 5, which further proves that the model can be used to simulate the effect of pore forming agent on matrix porosity.

Figure 6. SEM image of pore morphology with different amount of pore forming agent

(a) 50 μm  (b) 50 μm  (c) 50 μm  (d) 50 μm
5. Summary
In this paper, the phase field model is established based on the free energy function method. The M3/2/TiC cermet matrix is prepared by powder metallurgy method. The porosity of the matrix are measured to verify the phase field model. The experimental results show that the simulation value of porosity by phase field method is basically consistent with the experimental value, which proves that the phase field model can be used to simulate the effect of pore forming agent on the pore evolution process of matrix, which provides a basis for optimizing the preparation process of cermet matrix.

6. References
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