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ARTICLE

Numerical Simulation of Sintering of Non-equal Metal Powders by Surface Diffusion

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Abstract: This paper focuses on the numerical simulation of sintering of non-equal metal powders by surface diffusion. In order to simulate the sintering process of non-equal metal powders clearly, the surface diffusion model was modified by establishing more suitable initial boundary conditions. And this model was numerically solved by the finite difference method. The 2D and 3D numerical simulations of two metal powders with radii ratios of 1:1, 1:1.5, 1:2 were implemented by this model. Through comparison, the simulation results are consistent with the experimental ones. Finally, the effect of metal powders' radii ratios on the growth rate of sintering neck was investigated. The results show that the sintering neck radius increases with the decreasing of radii ratios of metal powders.

Key words: sintering; metal powders; surface diffusion; finite difference; radii ratio

Mass transport occurs at high temperature with a specific atmosphere. Surface diffusion, as a mass transport mechanism, plays an important role in sintering process of metal powders, metal fibers and grain-boundary grooves[1-5].

Sintering process have been extensively studied during the last decades[6-9], and many numerical methods have been used to simulate it, such as the MOL method[10], the finite element method[11], and the level set method[12]. The surface diffusion model, established by a nonlinear partial differential equation, was firstly proposed by Mullins[13]. For obtaining nearly flat surfaces, the small-slope limit was introduced to simplify the model. Subsequently, based on the seminal work of Mullins, many researchers concentrated on the symmetric model to numerically simulate the sintering process of grain-boundary grooves and metal powders[14-16], which means the investigation on the sintering process of symmetric system have been very mature. However, in the actual sintering process, the billet is usually composed of the powders with different dimensions. For solving this problem, some researches on the sintering process of non-symmetric model were proposed. Pan and Cocks[17] analyzed the coupled surface and grain-boundary diffusion for the non-isometric model. Zhang and Schneibel[18] investigated the sintering process of two equal and non-equal circular particles by surface and grain-boundary diffusion. Both in their research, the grain-boundary was assumed to be straight; however, the unbalanced total force in the perpendicular direction of the grain-boundary makes it impossible. Then, Du and Liang[19] adopted a non-isometric sintering model to deal with the initial sintering process and some fixed geometrical parameters were used in their research. Compared with the actual sintering process, the sintering junction and its neighboring points are constantly changing, which means that some geometrical parameters can not be fixed. In the previous numerical simulation, a fixed angle or some fixed geometrical parameters were used to deal with the boundary, which can not describe the sintering process of non-equal metal powders exactly. To date there is no perfect numerical simulation to solve the problem. Therefore, it

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is necessary to adopt a new boundary condition to describe the sintering process of non-equal metal powders clearly.

In this paper, combined the geometric structure of non-equal metal powders with the surface diffusion model, a new treatment of boundary condition was proposed. And the three-dimensional model of metal powders was developed to simulate the sintering process by surface diffusion. The 2D and 3D results of metal powders with different radii ratios were described. In addition, the effect of the metal powders' radii ratios on the growth of sintering neck was also investigated.

1 Mathematical Model

1.1 Geometric model

As shown in Fig.1, two metal powders have different radii R_1 and R_2, O_1 is the section of metal powder on the left, and O_2 represents the section of metal powder on the right. The two metal powders, with their neck radius Y, are inseparable throughout the sintering process due to mutual attraction.

1.2 Surface diffusion model

Surface diffusion results in mass flow along the materials surface and hence changes surface morphology[20]. According to the model derived by Mullins[13], mass transport by surface diffusion is driven by the gradient of chemical potential which is proportional to the surface flux. And the chemical potential on the surface is proportional to the curvature, so the surface flux is proportional to the gradient of curvature. In order to establish a reasonable model to describe the sintering process, the metal powders are regarded as spheres, and the surface diffusion is assumed to be the only mechanism responsible for surface movement. In this paper, only the incipient sintering process is studied, which means the radii of metal powders are nearly changeless.

In 2D case, the surface is represented by a curve. The mathematical model describing the surface movement introduced by Mullins[13] can be expressed as

$$\frac{\partial y}{\partial t}=-B\left\{\left(1+y_x^2\right)^{-1/2}\left[y_{xx}\left(1+y_x^2\right)^{-3/2}\right]_x\right\}_x \tag{1}$$

where B is a coefficient defined by

$$B=\frac{\delta_s D_s \gamma\, \Omega}{kT} \tag{2}$$

where D_S is the surface diffusion coefficient, γ is the surface free energy per unit area, Ω is the atomic volume, δ_S represents the surface diffusive width, k is the Boltzmann's constant and T is the absolute temperature.

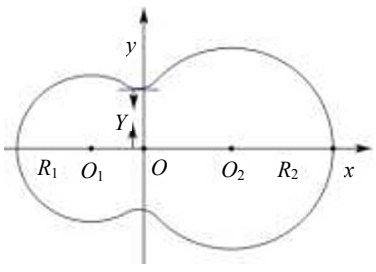

Fig.1 Geometric model of the non-equal metal powders

The function $y(x, t)$ is the surface profile with t representing time. The curvature of surface is

$$K=-\frac{y''}{\left(1+y'^2\right)^{3/2}} \tag{3}$$

which is positive for convex surfaces. The surface flux is defined as

$$J_s=-\frac{\delta_s D_s \gamma}{kT}\frac{1}{\left(1+y'^2\right)^{1/2}}\frac{\partial K}{\partial x} \tag{4}$$

The characteristic length scale in the sintering process is the initial radius of metal powders R. A dimensionless time $t^*=Bt/R^4$ and variables $K^*=RK$, $x^*=x/R$, $y^*=y/R$ are introduced. Substituting these dimensionless variables into Eq.(1) and Eq.(4), we have

$$\begin{cases}\dfrac{\partial y}{\partial t}=-\dfrac{\partial J_s}{\partial x}\\ J_s=-\dfrac{1}{\left(1+y'^2\right)^{1/2}}\dfrac{\partial K}{\partial x}\\ K=-\dfrac{y''}{\left(1+y'^2\right)^{3/2}}\end{cases} \tag{5}$$

According to the geometry of non-equal metal powders, if the boundary conditions of surface diffusion model are established, the numerical simulation on the sintering process of non-equal metal powders can be achieved.

1.3 Boundary conditions

The effect of surface diffusion is to make the sintering surface smooth. In the previous numerical simulation, a discontinuous point always exist at the sintering junction. For describing the sintering process more accurately, a new initial boundary condition is proposed. Let the sintering junction lie at $x=X$, using the superscripts '-' and '+' to indicate the left and right one-sided limits. In this numerical simulation, the surface at the junction is assumed to be continuous except the first time. The boundary conditions are as follows:

1) Two metal powders are inseparable throughout the sintering process due to mutual attraction. The continuity of the surface at the junction is

$$y(X^-,t)=y(X^+,t)=Y \tag{6}$$

2) In the initial state, two metal powders contact, the surface gradient is discontinuous at the junction, and the left and right one-sided limits are not equal. In this paper, at the first time, the sintering junction meets

$$y_x(X,0)=\frac{y_x^-(X,0)+y_x^+(X,0)}{2} \tag{7}$$

Subsequently, surface diffusion will make the curve profile smooth, the surface gradient becomes continuous, and this condition is still suitable.

3) At $x=-2R_1$, $2R_2$, according to the assumption by Mullins[13], at the edge of the system $J_S=0$. In this paper, the same hypothesis is implemented. And in the initial sintering process, the condition $y(-2R_1, t)=0$, $y(2R_2, t)=0$ are assumed.