A Modified Phase-Field Model for Non-Isothermal Sintering Induced by Local High-Temperature

Pengya Lei[1], Limin Li [1], Wenkui Yang [1], Hua Hou[1,3], Yuhong Zhao[1,2,4*]
1. School of Materials Science and Engineering, Collaborative Innovation Center of Ministry of Education and Shanxi Province for High-performance Al/Mg Alloy Materials, North University of China, Taiyuan, 030051, China
2. Beijing Advanced Innovation Center for Materials Genome Engineering, University of Science and Technology Beijing, Beijing, 100083, China
3. School of Materials Science and Engineering, Taiyuan University of Science and Technology, Taiyuan, 030024, China
4. Institute of Materials Intelligent Technology, Liaoning Academy of Materials, Shenyang, 110004, China
*Corresponding address: e-mail: zhaoyuhong@nuc.edu.cn

Abstract: The current isothermal sintering model cannot adequately describe the effect of local high-temperature on particle aggregation during spark plasma sintering (SPS), and a new non-isothermal sintering phase-field model suitable for spark plasma sintering is developed in this work. The model couples the heat conduction equation to the free energy to explore the impact of temperature on particle growth and observe its evolution mechanism. Using this model, the temperature not only affects the contribution of body energy by changing the temperature-dependent parameters but also significantly changes the gradient terms. When using this model to simulate non-isothermal sintering, we found that two identical particles grow asymmetrically under non-isothermal conditions, which is caused by the gradients of surface and grain boundary energies induced by local high-temperature. In addition, local high-temperature induces faster grain growth near the grain boundary, while the grain size in the center is smaller, which is confirmed in the experiment. The simulation results provide valuable insights for investigating particle growth under non-isothermal conditions.

Keywords:phase-field model, particle sintering, local high-temperature, temperature gradient, spark plasma sintering

1 Introduction

Solid sintering is widely used in powder metallurgy involving the applied heat and pressure to coalesce powder particles into a solid structure [1].The temperature is a critical parameter in the sintering process because it can act as a thermodynamic indicator and significantly affect the particles growth.

Although several studies on spark plasma sintering have been published in recent years, most of them regard the particles as a whole with uniform temperature without considering the influence of local high-temperature and temperature gradient on the particle evolution during sintering, which may lead to uneven temperature distribution inside the material, affecting the consistency and properties of the material. A new phase-field model for non-isothermal sintering is presented in this paper to observe the evolution of particle morphology under different temperature distributions, which is helpful in understanding the effect of temperature in the sintering process.

2 Phase field method

In a sintering system with multiple particles and pores, the total free energy F of the subdomain Ω within the system can be expressed as [2]:

$$F(T,\rho,\{\eta_\alpha\}) = \int_\Omega \begin{bmatrix} f(T,\rho,\{\eta_\alpha\}) + \frac{1}{2}T\kappa_\rho|\nabla\rho|^2 \\ +\frac{1}{2}T\kappa_\eta \sum_\alpha |\nabla\eta_\alpha|^2 \end{bmatrix} d\Omega \#(1)$$

Where the free energy density is:

$$f(T,\rho,\{\eta_\alpha\}) = f_{ht}(T)\left(A\rho + B\sum_\alpha \eta_\alpha\right) + C[\rho^2(1-\rho)^2] +$$

$$D\left[[\rho^2+6(1-\rho)]\sum_\alpha \eta_\alpha^2 - 4(2-\rho)\sum_\alpha \eta_\alpha^3 + \left(3\sum_\alpha \eta_\alpha\right)^2\right]\#(2)$$

$$f_{ht}(T) =- c_r T ln\frac{T}{T_0} + c_r(T-T_0)\#(3)$$

The modified temperature evolution equation is[3]

$$\frac{\partial T}{\partial t} = \mu\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right)\#(4)$$

3 Result and discussion

Particle agglomeration of two identical particles with temperature gradients

As shown in Fig 1(a), we apply a temperature gradient to two equal particles, which causes gradient changes in surface energy and grain boundary energy. The gradient between low and high temperatures creates a force that drives mass transfer, resulting in an uneven concentration distribution when non-isothermal particles gather. Thus, in this process, an asymmetric shape appears between two identical particles. Comparing the isothermal sintering process in Fig. 1(c), it can be found that temperature plays a dominant role in the process.

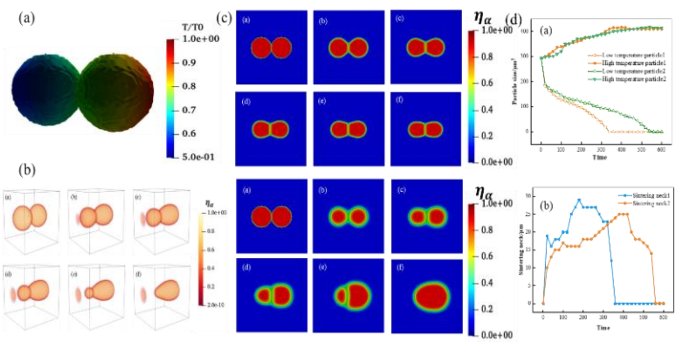

Fig. 1. (a) A three-dimensional diagram of two particles with a temperature gradient; (b) Three-dimensional results of particles evolution under temperature gradient; (c) Isothermal sintering and non-isothermal sintering particles evolution; (d) Under different temperature gradients, the particle area and the sintering neck on the cold side and the hot side evolves with time

Fig 1(d) shows the influence of different temperature gradients on the sintering process. The results show that the cold side particles and sintering neck disappear at the same time in the higher temperature gradient, which indicates that the higher temperature gradient will accelerate the sintering process.

Effect of local high-temperature on sintered grain size In the sintered particles, the particle size of each position in the initial stage is close, and there is no obvious difference in particle size. Due to the high local temperature at the grain boundary, the grain diffusion ability is strong and the annexation speed is fast. Therefore, at the later stage of sintering, the grains around the grain boundaries are significantly larger, while the particles in the center of the particles are smaller, as shown in Fig 2. The simulation results are in good agreement with the experimental results of AZ91D spark plasma sintering.

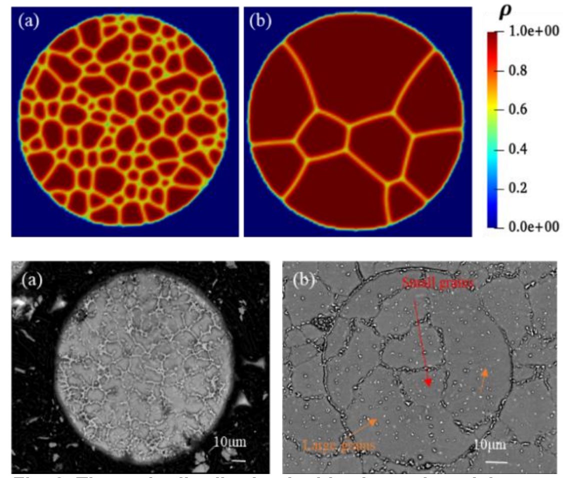

Fig. 2. The grain distribution inside sintered particles was observed by phase field simulation and experiment

4 Conclusion

In the sintering process of non-isothermal particles, the local high temperature of the gap causes the temperature gradient, and the gradient change of surface energy and grain boundary energy leads to the uneven distribution of the concentration of non-isothermal particles. At the same time, high temperature makes the grain at the grain boundary grow preferentially, so that the grain at the grain boundary is obviously larger than the grain at the core.

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References

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