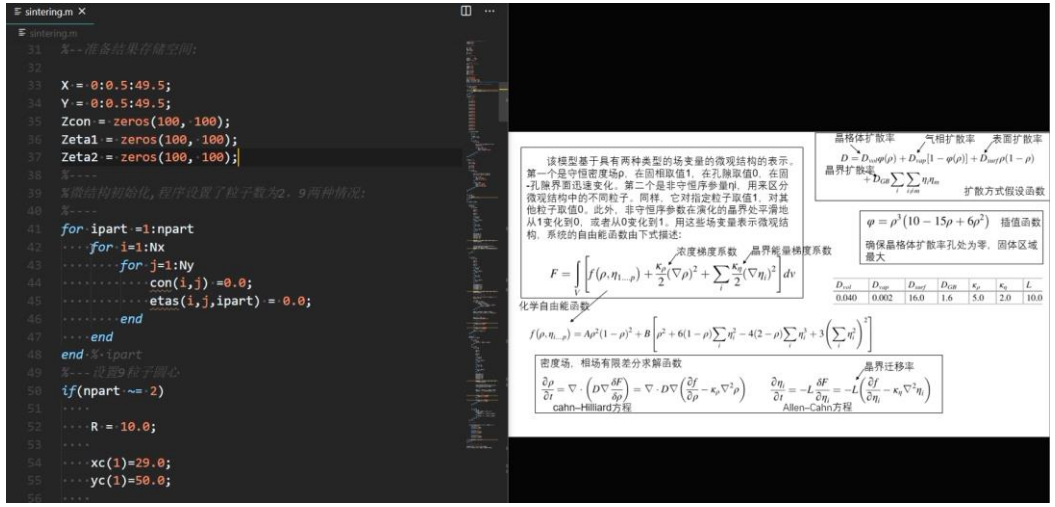
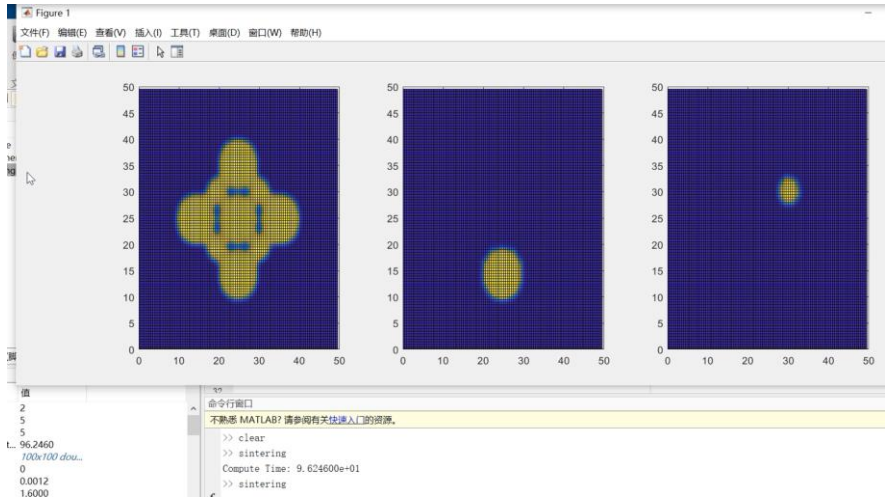
烧结过程的相场模拟

基于有限差分法的matlab实现





烧结是将粉末压块转化为致密固体的广泛使用的材料加工技术。从历史上看，它起源于古代的陶瓷加工。如今，它几乎是汽车和航空工业中微电子封装、纳米结构生产和网状零件制造的主要生产路线[1]。

烧结过程包括晶格间的体扩散、沿晶界的表面扩散、晶粒生长和晶界迁移、蒸汽传输(蒸发和冷凝)，以及最终粒子的刚性平移和旋转。

致密化和晶粒生长过程中严格控制孔隙率对于达到烧结材料所需的机械和物理性能至关重要。为了实现这些目标，实验并不总是足够的，需要对烧结这一过程进行数值模拟。

烧结过程模拟发展详细情况可通过参考文献[2-17]进行了解。

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Computer modeling and simulation of solid-state sintering: A phase field approach

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Abstract

A phase field model of solid-state sintering is developed. The model treats multiple concurrent physical processes, i.e., rigid-body translation and rotation of powder particles, grain growth through boundary migration, and various diffusion mechanisms including surface diffusion, grain boundary diffusion, volume diffusion, and vapor transport through evaporation and condensation. The approach of centers of particles through rigid-body motions plays a key role in the densification of sintered powder compacts. The effective treatment of particle translation and rotation in phase field formalism is a necessary and critical step in developing a phase field sintering model. A scheme of particle translation and rotation is formulated based on a new formula of grain boundary force. The rigid-body motion modifies both the Cahn–Hilliard nonlinear diffusion equation and the Ginzburg–Landau (Allen–Cahn) structural relaxation equation by introducing advection terms. Computer simulations are presented.

Keywords: Phase field model; Sintering; Diffusion; Grain boundary migration; Microstructure

Cahn–Hilliard方程

维基百科，自由的百科全书

所述**的Cahn-Hilliard方程**（后约翰·W·卡恩和约翰E. Hilliard的）是方程的数学物理描述的过程相分离，通过该二元流体自发地分离和形式的两种组分域在每个组件纯。如果c是流体的浓度，$c = \pm 1$表示域，则等式写为

$$\frac{\partial c}{\partial t} = D\nabla^2 \left(c^3 - c - \gamma \nabla^2 c\right),$$

哪里D是一个扩散系数，单位为$\text{Length}^2/\text{Time}$和$\sqrt{\gamma}$给出域之间过渡区域的长度。这里$\partial/\partial t$是偏时间导数，$\nabla^2$是拉普拉斯时代的$n$尺寸。另外，数量$\mu = c^3 - c - \gamma \nabla^2 c$被确定为化学势。

与之相关的是Allen–Cahn方程，随机Cahn–Hilliard方程和随机Allen–Cahn方程。

艾伦-卡恩方程

维基百科，自由的百科全书

所述**的Allen-卡恩方程**（后约翰·W·卡恩和Sam阿伦）是一个反应扩散方程的数学物理其描述了多组分合金系统，包括有序-无序转变的相分离的过程。

该方程式描述了标量值状态变量的时间演化η在域上Ω在一个时间间隔内$\mathcal{T}$，并由：[1] [2]

$$\frac{\partial \eta}{\partial t} = M_\eta[\operatorname{div}(\varepsilon_\eta^2 \nabla \eta) - f'(\eta)] \quad \text{on } \Omega \times \mathcal{T}, \quad \eta = \bar{\eta} \quad \text{on } \partial_\eta \Omega \times \mathcal{T},$$
$$-(\varepsilon_\eta^2 \nabla \eta) \cdot m = q \quad \text{on } \partial_q \Omega \times \mathcal{T}, \quad \eta = \eta_o \quad \text{on } \Omega \times \{0\},$$

哪里M_η是流动性f是双阱潜力，$\bar{\eta}$是对边界部分的状态变量的控制$\partial_\eta \Omega$，q是位于的源代码控制$\partial_q \Omega$，η_o是初始条件，并且m是外向法线$\partial\Omega$。

它是金茨堡-朗道自由能泛函的L^2梯度流。[3]它与Cahn-Hilliard方程密切相关。

该模型基于具有两种类型的场变量的微观结构的表示。第一个是守恒密度场ρ，在固相取值1，在孔隙取值0，在固-孔隙界面迅速变化。第二个是非守恒序参量ηi，用来区分微观结构中的不同粒子。同样，它对指定粒子取值1，对其他粒子取值0。此外，非守恒序参数在演化的晶界处平滑地从1变化到0，或者从0变化到1。用这些场变量表示微观结构，系统的自由能函数由下式描述:

浓度梯度系数　晶界能量梯度系数

$$F = \int_V \left[f(\rho, \eta_{1\ldots p}) + \frac{\kappa_\rho}{2}(\nabla\rho)^2 + \sum_i \frac{\kappa_\eta}{2}(\nabla\eta_i)^2 \right] dv$$

化学自由能函数

$$f(\rho, \eta_{i\ldots p}) = A\rho^2(1-\rho)^2 + B\left[\rho^2 + 6(1-\rho)\sum_i \eta_i^2 - 4(2-\rho)\sum_i \eta_i^3 + 3\left(\sum_i \eta_i^2\right)^2\right]$$

晶格体扩散率　气相扩散率　表面扩散率

$$D = D_{vol}\varphi(\rho) + D_{vap}[1-\varphi(\rho)] + D_{surf}\rho(1-\rho)$$

晶界扩散率

$$+ D_{GB}\sum_i \sum_{i\neq m} \eta_i\eta_m$$

扩散方式假设函数

$$\varphi = \rho^3(10 - 15\rho + 6\rho^2)$$　插值函数

确保晶格体扩散率孔处为零，固体区域最大

D_{vol}	D_{vap}	D_{surf}	D_{GB}	κ_ρ	κ_η	L
0.040	0.002	16.0	1.6	5.0	2.0	10.0

密度场，相场有限差分求解函数

晶界迁移率

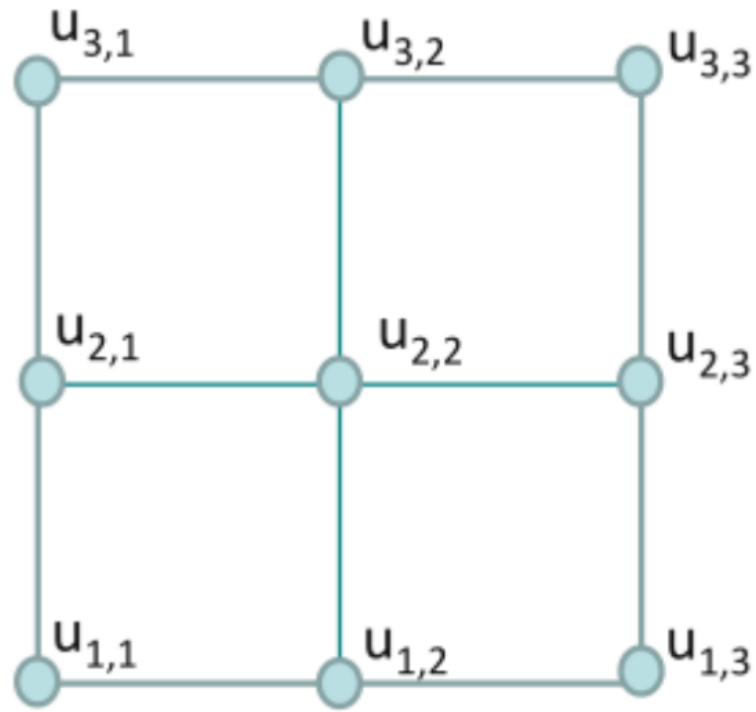
$$\frac{\partial\rho}{\partial t} = \nabla\cdot\left(D\nabla\frac{\delta F}{\delta\rho}\right) = \nabla\cdot D\nabla\left(\frac{\partial f}{\partial\rho} - \kappa_\rho\nabla^2\rho\right)$$

cahn–Hilliard方程

$$\frac{\partial\eta_i}{\partial t} = -L\frac{\delta F}{\partial\eta_i} = -L\left(\frac{\partial f}{\partial\eta_i} - \kappa_\eta\nabla^2\eta_i\right)$$

Allen–Cahn方程

$$\left(\nabla^2 u\right)_{i,j} = \frac{u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}}{h^2}$$



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