



Phase field modeling of sintering: Role of grain orientation and anisotropic properties

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ABSTRACT

The influence of anisotropic properties of powder particles on microstructural evolution during solid-state sintering processes is analyzed. Two types of anisotropy studied in the current work are direction-dependent interface diffusion anisotropy, and grain orientation dependent grain boundary energy anisotropy. A phase field modeling approach is utilized to assess how the individual anisotropic characteristics influence morphological changes during sintering. In addition, a novel approach for updating grain orientation after rigid-body rotation of particles during powder compaction accompanying the sintering process is developed. It is observed that conventional isotropic microstructural analysis over-simplifies the material behavior and demonstrates faster microstructural evolution. Direction-dependent diffusion produces gradual shape change of the particles by mass transfer from high curvature region to low curvature region along the particle surface, and delays the onset of the grain growth process. Depending on the grain boundary misorientation and inclination, anisotropic grain boundary energy may induce faster or slower grain boundary migration rate. Orientation update during the process plays a critical role in the consolidation kinetics, as well as in the final microstructural configuration. Variation in grain orientation and its evolution during the sintering process can produce different grain morphologies for the same initial condition.

1. Introduction

Sintering is a material processing technique for coalescing powder materials into a solid structure by applying external pressure and heat. This process has been proven to be beneficial in several applications, especially for materials having low bonding energies or high melting points. It has been adopted in various manufacturing and material processing industries to process ceramics, semiconductors, as well as some metals [1–4]. Conventionally, sintering is studied through experiments to assess the morphological changes during the process. Several researchers have studied different sintering techniques to observe how variations in individual process parameters influence the consolidation kinetics during the process and produce different microstructural textures. For example, Grigoryev [5] has shown external process parameters such as electric discharge and pressure affect densification kinetics and produce improved material density. Hu et al. [6] have shown that a higher heating rate yields higher rate of densification, while lower heating rates provide higher relative density. Alexander and Balluffi [7] have shown that during sintering of Cu wires bonding between two particles in the early stages is initiated due to

surface diffusion, whereas the particle shrinkage throughout the process is a result of volume diffusion of atoms from the grain boundary (GB).

Apart from the experimental studies, several computational [8–10] and analytical [11–14] models have been developed to evaluate role of different process parameters during the sintering process. It has been observed that there are three distinct stages of sintering involving neck formation and grain growth. However, in order to determine how each mechanism influences the shape and size change of the particles during different stages of sintering, *in-situ* examination is required. Very little work has been done in this regard, as developing *in-situ* sintering experiment is very expensive. A relatively inexpensive way of observing microstructural changes during the process is through simulations. The present work offers a framework to study sintering using phase field modeling (PFM). Chen, Hassold and Srolovitz [15,16] developed a Monte Carlo simulation model to predict microstructural changes and sintering mechanisms during the final stages of sintering. They also evaluated the influence of initial pore size and captured the pore behaviors during the sintering process. Tikare et al. [17] applied Pott's Kinetic Monte Carlo (KMC) model to understand the characteristics of

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powder compaction during solid state sintering of complex powder particles in 3D. The model was shown to be able to identify different microstructural features such as necks, pores, etc. created during the process and demonstrate different stages of sintering. Braginsky et al. [13] used the same model to establish how different diffusion mechanisms affect the overall deformation behavior during the sintering process. Nevertheless, due to the stochastic nature of the KMC, of late, several other researchers are adopting diffuse interface based PFM approach for capturing microstructural evolution during sintering.

Wang [18] was the first to propose a PFM model that captures mechanisms behind the sintering process. He also proposed the rigid body motion formulation required for simulating powder compaction during the sintering process. Later, Kumar et al. [19] used the same approach to study different sintering stages during compaction of unequally sized particles. Shinagawa [20] combined PFM with a discrete element method to capture the GB migration and shrinkage. They have also proposed the limits and methods to select free energy coefficients and mobility parameters for such PFM simulations. However, all of the models assume the material properties to be isotropic. In reality, however, most materials are not isotropic and within a single material, properties can vary spatially depending on the microstructural features. For example, different grains can have independent crystallographic orientation or diffusion in a specific direction can be higher than other directions. Anisotropic properties introduced by all such factors are very important in predicting realistic material behavior from simulations. The role of anisotropic interface properties and misorientation in several phase transformation scenarios such as solidification, grain growth etc. have been studied for some time now. Kobayashi [21] first introduced anisotropy in dendritic growth which occurs during solidification or crystallization of materials. It has been shown that anisotropy not only affects the equilibrium shape of a crystal or phase, it also affects the growth pattern. This model has been further extended to study the dynamics of GB formation and its evolution during solidification of a polycrystalline material [22,23]. The role of misorientation has also been considered to predict anisotropic grain growth behavior using KMC simulations [24,25] and a PFM approach [26–29]. Kazaryan [30] was the first to come up with a simplistic approach for anisotropic grain growth that demonstrated the significance of the GB energy anisotropy as well as the mobility anisotropy considering dependence of anisotropic properties on both misorientation between the grains and GB inclination. Upmanyu et al. [31] compared the importance of energy and mobility anisotropy during normal grain growth using both KMC and PFM approaches. Both analyses indicate grain growth kinetics is insensitive to mobility anisotropy, whereas small GB energy anisotropy can produce anisotropic grain shapes and strong texture. Although anisotropic properties are known to influence microstructural evolution in different scenarios, very limited work has been done to take into account such behavior for sintering simulations.

Deng [32] implemented direction dependent diffusion parameters in a PFM model to capture realistic shape changes and interface formations during the sintering process. According to their predictions, the consideration of direction dependent mobility brings the diffuse interface model close to the sharp interface approach and can depict the neck formation behavior between two particles having complex shapes. Ahmed et al. [33] adopted a similar model to study grain growth in a porous media and as a test case applied the model to analyze sintering of two unequal size particles. However, a discussion on how the mechanisms predicted from the model are different from isotropic case is missing. Moreover, none of the previous work considered the role of grain orientation on the grain morphology changes during the sintering process and role of anisotropic properties, especially dependence on misorientation and GB inclination in the case of sintering simulation. In this work, how different anisotropic property considerations affect morphological changes during the sintering process is illustrated. The current work focuses on incorporating anisotropic properties to the PFM previously developed by Biswas et al. [34,35]. Primary

developments are concentrated on quantifying the role of anisotropic properties on the densification mechanisms at different stages of sintering. The role of grain orientation on GB formation and its evolution/migration is studied. Moreover, during sintering the particles can translate or rotate as a rigid body and this rigid-body rotation changes the crystallographic orientation of the grains. This unique characteristic is considered for the first time and an algorithm for updating the grain orientation with each rotation is developed. The organization of the paper is as follows: First, in Section 2, a formulation for the PFM along with modifications done to incorporate anisotropic behavior is presented. A method for updating grain orientation after any rigid-body rotation of the particle is described. In Section 3, simulation results illustrating role of anisotropic mobilities and misorientation of the neck formation and grain growth during the sintering process are presented. Finally, in Section 4, conclusions are discussed from the study, highlighting the importance of the consideration of anisotropic properties during such simulations.

2. Modeling approach and formulation

In the phase field model presented here, the microstructure of the powder material is represented with a conserved and a nonconserved variable. The concentration of the powder particles (c) is taken as the conserved variable, which has a value of one inside a particle and zero everywhere else. The nonconserved variables (η_i) are associated with the crystallographic orientation of each particles such that $\eta_i = 1$ inside the i^{th} particle and 0 otherwise. In this study, individual particles are assumed to have single-crystalline structures, polycrystalline particles are beyond the scope of this paper. Details of the basic phase field model with isotropic properties used for sintering has been reported in the author's previous works [35,36]. In this section, a brief description of the model and the details about incorporating anisotropic properties is provided.

For the phase field approach, the total free energy (F_{total}) of the system is represented as

$$F_{total} = \int \left[f(c, \eta_i) + \frac{1}{2} \kappa_c |\nabla c|^2 + \frac{1}{2} \sum_i \kappa_{\eta_i} |\nabla \eta_i|^2 \right] dV. \quad (1)$$

The first term within the integral represents the bulk free energy density of the system due to its constituent phases. The second and third gradient terms denote the excess interfacial energy at the interface between the particle/void phase and the grain boundaries, respectively. The bulk free energy [18,34,35] is expressed in terms of the phase field variables as

$$f(c, \eta_i) = A c^2 (1-c)^2 + B \left[c^2 + 6(1-c) \sum_i \eta_i^2 - 4(2-c) \sum_i \eta_i^3 + 3 \left(\sum_i \eta_i^2 \right)^2 \right], \quad (2)$$

where,

$$A = \frac{(12\gamma_s - 7\gamma_{GBij})}{\delta}, \text{ and} \quad (3)$$

$$B = \frac{\gamma_{GBij}}{\delta}, \quad (4)$$

are the bulk free energy coefficients that are calculated based on the GB and surface energy (as proposed by Ahmed et al. [33] of the materials. Here, γ_s and γ_{GBij} are the surface energy and GB energy between i^{th} and j^{th} grain, respectively. The gradient energy coefficients (κ_c , κ_{η_i}) are obtained as

$$\kappa_c = \frac{3}{4} \delta (2\gamma_s - \gamma_{GBij}), \text{ and} \quad (5)$$

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