Computational Materials Science 143 (2018) 338–349

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Combining densification and coarsening in a Cellular Automata-Monte-Carlo simulation of sintering: Methodology and calibration

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ARTICLE INFO

Article history:
Received 25 July 2017
Received in revised form 10 November 2017
Accepted 11 November 2017
Available online 24 November 2017

Keywords:
Sintering
Densification
Modelling
Microstructure evolution
Cellular automata
Monte-Carlo

ABSTRACT

A hybrid Cellular Automata-Monte Carlo (CA-MC) approach is developed to simulate the sintering of particulate materials. The approach embodies a new, and physically realistic, way of simulating densification by grain boundary diffusion and collapse that takes into account the stresses arising from interactions with neighbouring particles (grains) by minimising the stored energy and energy dissipation rate using the variational principle. The parameters in the CA-MC simulations are calibrated in terms of measurable physical quantities by simulating the sintering of two identical contacting spheres, for which analytical solutions are well known and widely accepted. The use of the model is illustrated by simulating the densification of a randomly packed assembly of spherical particles. This demonstrates that the interactions between particles significantly inhibits shrinkage compared with that of two isolated spheres.

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1. Introduction

Sintering of assemblies of particulates (such as powder compacts) involves both coarsening and densification driven by the excess energy of solid/pore interfaces. Surface diffusion, from positions of high curvature to positions of low curvature, leads to coarsening without densification. In crystalline materials densification is caused by diffusion from grain boundaries to positions of low curvature and subsequent collapse (annihilation of vacancies) at the grain boundary bringing the grain centres closer together. Theoretical modelling plays an important role in improving understanding of the sintering process. Originally, sintering theory concentrated on simple two-sphere models [1–5] with one neck formed between two identical spherical particles. Despite the simplification, these models were successful in providing fundamental understanding about the sintering driving force and the transport processes controlling the kinetics of neck growth and shrinkage.

The initial morphology and topological features of real microstructures, and their evolution during sintering are much more complicated than is assumed in most simulation methods described in the literature. For example, it has been observed experimentally [6] that the faceted surfaces of particles can lead to neck growth kinetics that are significantly different from the predictions of classic continuum theory (which is based on idealised spherical particles). Therefore there is a clear need to include the evolution of more realistic microstructural features during the simulation of sintering [7].

Although useful for fundamental insight, two-sphere models cannot describe the macroscopic behaviour of a typical powder compact, in which multi-particle interaction occurs, involving thousands to millions of particles having different shapes, sizes and arrangements. To try and tackle this, micromechanical models [5,8,9] based on periodic unit cells were developed, which described the macroscopic viscous behaviour of a powder compact based on information such as starting particle size and/or pore size, particle coordination and fundamental parameters such as diffusion coefficients for different matter transport pathways. However constitutive parameters obtained in these models are rather approximate as they are obtained from analytical solutions for highly simplified grain and pore structures (mostly spherical or cylindrical) [7]. More recently the discrete element method (DEM) has been developed to take multiple particle-particle interactions into account. This approach has been used particularly in modelling constrained sintering [10–15]. It uses the analytical model for sintering of a pair of spherical particles to calculate the forces acting on any given pair in the assembly of particles and then computes their consequent rigid motion [16]. A key feature of the DEM method is that it models the response of typically tens of thousands of particles and is therefore well-suited to simulating semi-macroscopic behaviour. It has been successfully applied to

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https://doi.org/10.1016/j.commatsci.2017.11.023
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simulate the development of anisotropic microstructure during sinter forging [14], shape distortion and delamination during constrained sintering of ceramic strips [17] and defect evolution (e.g. cracks) in sintering [12]. However, the DEM method requires that the particles are initially spherical and that densification can be simulated by the interpenetration of the initial spheres and described quantitatively by the two-sphere sintering model. Consequently, the initial spherical solid portions that have not overlapped during densification are retained in the evolving microstructure. Hence the approach is suitable for simulating only the early and intermediate stages of sintering. Particle coarsening and shape changes of solid surfaces and pores, which are extremely important in understanding the detailed microstructure development, and sintering in the later stages, are not included.

The phase field method is capable of modelling real complicated microstructural changes for a wide variety of material processes [18–20]. However a realistic phase field model of sintering including densification is yet to be developed. The obstacle hindering the phase field approach to sintering is associated with the difficulty in treating the particle rigid body motions in an effective way consistent with phase field formalism [20,21].

Cellular automata (CA) [22–24] and Monte-Carlo (MC) [7,25–32] methods can be used to model evolution of any complicated microstructure without prohibitive computation cost. In these methods space is discretised into cells (or voxels in 3 dimension). The state of any given cell is allowed to change with advancing time (e.g. from one grain orientation to that of a neighbouring grain if simulating grain growth) determined by simple switching rules. This mimics what happens in reality on an atomistic level and therefore reflects the fundamental energy driving forces and kinetic mechanisms underpinning the microstructure changes. One major advantage of this approach is that both CA and MC have the capability of modelling multiple processes acting simultaneously. For example curvature-driven grain growth and coarsening by surface transport acting in parallel can be taken into account in a CA and MC model [30,32,33].

Previously we have used the CA approach in simulating the evolution of the 2D microstructure of materials [23] and the 3D microstructure degradation of nickel/zirconia cermet fuel cell electrodes [22] by evaporation-condensation and grain growth. The CA models have also been shown to reproduce well known phenomena such as wetting, grooving and particle coarsening. Quantitative relationships have been established in those studies between modelling parameters and wetting angle and grain boundary groove angle [23].

However, the potential benefits of CA and MC methods have not yet been fully explored or exploited in sintering. In particular, the process of grain boundary diffusion and resulting grain boundary collapse that leads to densification has not been implemented in the CA-MC approach. This, and calibration of the model parameters in terms of real physical quantities, are necessary to simulate microstructure evolution during sintering of particle assemblies.

In this paper, we first extend our CA-MC simulation approach to matter transport in a sintering body by surface diffusion. We then develop a physically realistic CA-MC methodology to deal with grain boundary diffusion and collapse (which is responsible for densification) that takes into account the effect of shrinkage mismatch, among different neck-connected particle pairs, on the rigid body motion of particles using the variational principle. To the best of our knowledge, this is the first time that a sintering model can not only account for multiple mass transport mechanisms and deal with real microstructure without simplification, but also treat grain boundary collapse appropriately. The simulations of individual processes (corresponding to different mass transport mechanisms) are calibrated against classical continuum theories using the well-studied two-sphere case. This allows us to establish the quantitative relationship between the CA-MC model parameters and fundamental physical parameters such as surface and grain boundary diffusion coefficients. Finally, we illustrate the use of the methodology by applying it to the sintering of a randomly packed assembly of spherical particles.

2. Methodology

2.1. Energy functions and state switching

In both CA and MC, space is discretised as cells. Each cell is assigned an internal state describing its nature (e.g. solid, pore, surface, interface, crystal orientation) and its internal energy with respect to a common reference energy. The system evolves by the exploring switching the state of the cells according to an energy-based criterion or set of rules. The energy of a given cell depends on its interaction with neighbouring cells which we term "structural imbalance" [22,23]. In CA, all the cells that are in a position to make a switch to a lower energy state are allowed to switch their state simultaneously (within one time-step). This is applicable to some physical processes (such as evaporation-condensation and grain boundary migration) where the probability of a cell's state switch can be assumed to be independent of the outcome of its neighbour's state switch. When simultaneous state switching cannot be applied (e.g. for grain boundary diffusion and collapse, or surface diffusion) the MC approach is used to decide whether a state switch occurs. When MC is used, one relevant cell is chosen randomly for a decision regarding a state switch. Therefore, time in the MC model is measured in units of a "Monte Carlo step" (MCS) which corresponds to N attempted changes (or substeps), where N is the total number of relevant cells.

During sintering, the driving force for matter transport is the free energy change associated with surface curvature. In the classical continuum theories (e.g. Gibbs-Thomson equation) the excess free energy is related to curvature as $\Delta G \propto 1/r_c$ (where r_c is the local radius of curvature). Curvature is a macroscopic concept which is simple, accurate and elegant in dealing with surface/interface energy problems. While the classic Gibbs-Thomson equation is convenient to apply in 2 dimensions or to a sphere, for 3-D non-spherical surfaces a generalized Gibbs-Thomson equation [34] may be used with the two principal curvatures in orthogonal directions $1/r_c = 1/r_1 + 1/r_2$. Johnson's generalized Gibbs-Thomson equation [34] is simple in form but not computationally efficient to apply. Furthermore, the concept of curvature only applies to smooth surfaces and cannot deal with sharp features or edges. Therefore, in order to develop a generally applicable method for computer simulation, it is necessary to use a concept which is not only physically equivalent to curvature for smooth surfaces, but is also computationally more efficient. In our earlier papers we have demonstrated that the concept of "structural imbalance" accurately represents the local energy increase due to the presence of non-balanced bonding at a surface or interface [22,23] (i.e. bonding that is different from that in the homogeneous bulk material). The quantified structural imbalance of surface and interface voxels is consistent with the local 'curvature' (the concept used in classical continuum theories) in describing the local energy increase. By using this concept of structural imbalance, interface wetting, grain boundary grooving and grain growth can all be reproduced accurately using cellular automata approach [22,23]. The concept of energy change due to curvature is thus one way of describing structural imbalance for a smooth surface. Furthermore, the concept of structure imbalance is more generally applicable in dealing with interface energy problems. It can easily accommodate anisotropic surface/interface energies and complicated geometrical features into quantification.

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