Simulation Modelling Practice and Theory 62 (2016) 102–116

Contents lists available at ScienceDirect

Simulation Modelling Practice and Theory

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

Numerical simulation of a coupled nonlinear model for grain coarsening and coalescence

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ARTICLE INFO

Article history:
Received 30 October 2014
Revised 21 January 2016
Accepted 24 January 2016
Available online 20 February 2016

Keywords:
Grain coarsening
Grain coalescence
Kinetic nonlinear model
Differential equation
Mass transfer simulation algorithm
Ostwald ripening

ABSTRACT

A kinetic nonlinear model of mass transfer, grain coarsening and coalescence with potential applications in sintering processes is studied. The model involves nonlinear ordinary differential equations that determine the transport of mass between grains. The rate of mass transfer is controlled by an Arrhenius factor leading to a nonlinear model of mass transfer and grain coarsening. The resulting dynamical system of coupled nonlinear differential equations with random initial conditions (i.e., initial grain mass configuration) is solved by means of the fourth order Runge–Kutta method. We conduct an analysis of the two-grain system and identify three dynamic regimes (diffusive, growth-decay and trapping). The same regimes are shown to persist in the multigrain system. We confirm the numerical performance of the Runge–Kutta method by means of a suitable convergence measure. The influence of the activation energy parameter on the dynamic regimes is investigated. It is shown that as the parameter grows the diffusive regime is progressively restricted to smaller values of the initial grain distribution. We introduce grain coalescence in the mass transfer equations, and we show that it accelerates the growth of the larger grains. Finally, we compare the dynamic evolution of the grain size distribution with the Ostwald ripening expression.

1. Introduction

Many technological materials, including ceramics, are produced by means of nonequilibrium physical processes that generate phase changes. A typical example is sintering, a process during which a powder is transformed into a monolithic material through atomic diffusion mechanisms. The modeling of sintering is a long-standing problem which remains poorly understood to date. Early studies of phase change kinetics have focused on interactions between grains that produce a crystal aggregate [1,2]. Recent approaches use the Discrete Element Method (DEM) to relax assumptions regarding the particle kinematics [3,4]. In DEM, grain coarsening is accounted by considering the overlapping volume of neighboring spherical particles, increasing the radius of the larger particle while decreasing the radius of the smaller by the same amount. By applying temperature and pressure the process of solid state sintering transforms a powder into a monolithic material [5].

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http://dx.doi.org/10.1016/j.simpat.2016.01.012
S1569-190X(16)00019-8/

Nomenclature

$m_i(t)$	mass of ith grain at time t (dimensionless units)
N	number of grains
$u = \alpha Q/N_A K_B T$	dimensionless grain activation energy
α	dimensionless rate factor
Q	characteristic activation energy
N_A	Avogadro constant
K_B	Boltzmann's constant
T	temperature
δ	coalescence control parameter
$r_i(t)$	radius of ith grain (dimensionless units)
ρ	mass density of the grains—assumed to be constant (dimensionless units)
N_s	total number of simulation steps
Δt	time step
t_f	final simulation time
K_c	number of simulation steps between coalescence tests

Sintering involves diffusion and transport of atoms as well as plastic deformations. During the sintering process, the number of grains is reduced, whereas the average grain radius increases. Such process is known as Ostwald ripening [6,7].

Modeling the sintering kinetics is a topic of continuing research. Recent computational techniques involve the Direct Multiscale Modeling [8], the DEM [3,4] and generalized Monte Carlo simulations [9]. In DEM, grain coarsening is incorporated by transferring the overlapping volume of neighboring spherical particles from the smaller to the larger. Grain coarsening is also observed in diffusion processes such as the Cahn-Hilliard equation [10] that describes phase separation (reverse diffusion), and the phase-field models used in solidification [11]. Recently, a self-consistent, mean-field kinetic theory has been proposed to describe atomic diffusion in non uniform alloys [12].

The grain coarsening observed during sintering provides the motivation for this work. Our ultimate goal is to use the proposed model to predict the impact of key sintering parameters such as time and temperature as well as the powder grain size distribution and the activation energy on the final grain size distribution. Herein we investigate numerically a one-dimensional, nonlinear kinetic model of mass transfer, grain coarsening, and coalescence, which significantly extends the scope of the original model introduced in [13]. The model comprises a system of nonlinear ordinary differential equations (ODEs) and incorporates local fluctuations in mass transfer rates due to variations in the degree of grain amorphization. The initial conditions for the system are grain masses which are considered to be randomly distributed. The new contributions of this manuscript are briefly described below. We solve the initial value problem by means of the fourth-order Runge–Kutta method and compare the results with the explicit Euler scheme. We confirm the numerical performance of the two methods and the superiority of the Runge–Kutta method by studying suitable convergence measures. A detailed analysis of the two-grain system is presented, which leads to the identification of three dynamic regimes that include diffusion, growth-decay (reverse diffusion) and trapping. The first two regimes may be related, respectively, to the normal and abnormal growth regimes observed in [16]. Similar behavior is also observed in numerical solutions of the multigrain system. We also introduce a grain coalescence mechanism and study its impact on the evolution of the grain size distribution. Finally, we compare the dynamic evolution of the grain radii with the Ostwald ripening theoretical expression.

This manuscript is organized as follows. In Section 2 we present the nonlinear kinetic model of mass transfer between grains. The model comprises a system of nonlinear ordinary differential equations that allow the exchange of mass between grains. The grains are arranged along a line (open boundary conditions) or along a ring (periodic boundary condition). The initial values of the grain masses are random numbers drawn from the normal, lognormal or some empirical probability distribution. Section 3 is devoted to the analysis of the two-grain system, in particular a discussion of the different evolution regimes in the system. Numerical solution of the multigrain system using the Runge–Kutta method and comparison of the numerical results with the explicit Euler scheme is presented in Section 4. A computational algorithm involving grain coalescence technique is described in Section 5. Section 6 focuses on a numerical simulation of the multigrain system in which we permit coalescence of two neighboring grains based on their mass contrast. Numerical examples are illustrated. Here we also discuss about limitations and assumptions of the proposed techniques. Section 7 discusses the results obtained with the mass transfer model in relation to Ostwald ripening. Section 8 presents our conclusions and suggestions for further work based on the limitations of the current approach.

2. Nonlinear kinetic model

An ensemble of spherical grains is considered such that the surface of each grain (particle) is in contact with its nearest neighbors. We study a one-dimensional geometry in which N grains are located along a line, and each grain has two