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Kinetic model of mass exchange with dynamic Arrhenius transition rates



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HIGHLIGHTS

- We investigate a non-equilibrium model of mass exchange with nonlinear dependence of transfer rates.
- We established diffusive and growth–decay regimes.
- A trapping effect was observed which can impede mass evolution in both regimes.
- We found that the dynamic regime depends on the activation parameter and initial mass distribution.
- Lower values of the activation parameter (i.e., higher values of temperature) favor the diffusive regime.

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ABSTRACT

We study a nonlinear kinetic model of mass exchange between interacting grains. The transition rates follow the Arrhenius equation with an activation energy that depends dynamically on the grain mass. We show that the activation parameter can be absorbed in the initial conditions for the grain masses, and that the total mass is conserved. We obtain numerical solutions of the coupled, nonlinear, ordinary differential equations of mass exchange for the two-grain system, and we compare them with approximate theoretical solutions in specific neighborhoods of the phase space. Using phase plane methods, we determine that the system exhibits regimes of diffusive and growth–decay (reverse diffusion) kinetics. The equilibrium states are determined by the mass equipartition and separation nullcline curves. If the transfer rates are perturbed by white noise, numerical simulations show that the system maintains the diffusive and growth–decay regimes; however, the noise can reverse the sign of equilibrium mass difference. Finally, we present theoretical analysis and numerical simulations of a system with many interacting grains. Diffusive and growth–decay regimes are established as well, but the approach to equilibrium is considerably slower. Potential applications of the mass exchange model involve coarse-graining during sintering and wealth exchange in econophysics.

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1. Introduction

Non-equilibrium processes such as grain growth and nucleation remain a topic of interest in statistical physics [1]. Such phenomena are common in many engineering and physical processes [2]. A grain is defined as a contiguous region of material with the same crystallographic orientation which changes discontinuously at the grain boundaries. Many

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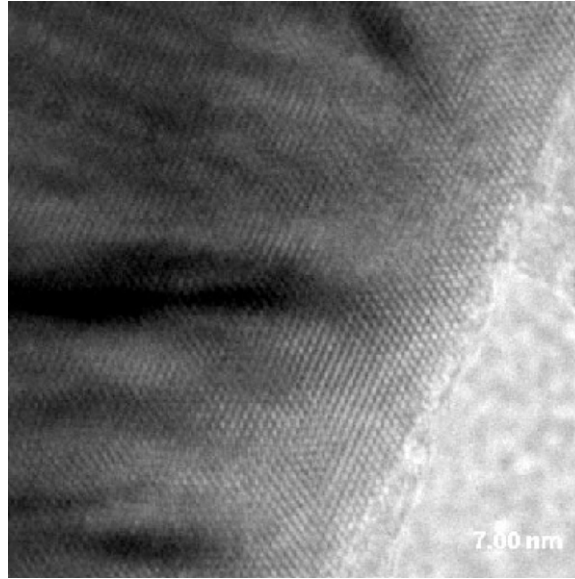


Fig. 1. High resolution Transmission Electron Microscope (HRTEM) image of mechanically activated alpha-silicon nitride grain. The image is provided courtesy of Prof. Malgorzata Sopicka-Lizer, Silesian University of Technology, Poland.

technological materials, including advanced ceramics, are produced by means of non-equilibrium physical processes that generate phase changes and grain growth. Early studies of the kinetics of crystallization and other phase changes were based on the Johnson–Mehl–Avrami–Kolmogorov equation [3,4]. The process of solid-state sintering transforms a powder into a monolithic material by applying temperature and pressure [5]. Sintering involves diffusion and transport of atoms as well as plastic deformations. During the sintering process, the number of grains is progressively reduced, while the average grain radius increases in a process known as Ostwald ripening [6,7].

Whereas sintering is essentially a simple process of densification by heating, its details are complicated. Hence, modeling the sintering kinetics is a topic of continuing research. Recent computational approaches involve Direct Multiscale Modeling [8] and the Discrete Element Method (DEM), which relax assumptions regarding the particle kinematics [9,10] and generalized Monte Carlo simulations [1]. In DEM, grain coarsening is incorporated by transferring the overlapping volume of neighboring spherical particles from the smaller to the larger. Existing sintering models are continuum formulations. This is also true of diffusion processes such as the Cahn–Hilliard equation [11], which describes phase separation (reverse diffusion), and the phase-field models used to describe solidification [12]. Recently, a self-consistent, mean-field kinetic theory was proposed to describe atomic diffusion in non-uniform alloys [13]. This theory uses thermally activated transition rates between species and corrects the Cahn–Hilliard model in the presence of non-uniformities.

Mass diffusion during sintering is controlled by an activation energy which can be lowered by means of ball milling [14]. A high resolution transmission electron microscope image of an alpha-silicon nitride grain (an alloy based on silicon nitride, Si_3N_4 , in which some silicon atoms are replaced by Al and corresponding Ni atoms by O) after mechanical activation by ball milling is shown in Fig. 1. The grain includes areas with both oriented and disordered lattice structure which occur both inside and near the boundary of the grain. This structure can lead to both intra-grain and inter-grain diffusion.

Motivated by the above observations, we study a simplified model of mass exchange between grains. The exchange is governed by a kinetic equation which involves transition rates that are based on the Arrhenius equation $k = \exp(-E_a/k_B T)$, where k is the rate coefficient (reaction constant), E_a is the activation energy, k_B is Boltzmann’s constant, and T is the temperature. The kinetic model that we study herein is too simple to accurately capture properties of the actual sintering process. Nevertheless, it exhibits a notable transition between a diffusive regime in which the equilibrium grain masses tend to become equal, and a growth–decay (reverse diffusion) regime in which the larger mass grows whereas the smaller one shrinks. These two distinct regimes may be related, respectively, to normal and abnormal growth regimes observed in sintering [15].

1.1. Nonlinear mass exchange model

In Ref. [16] we introduced a kinetic model for mass exchange between N grains of different radii. The model involves a system of N coupled, non-linear, ordinary differential equations (ODEs) with Arrhenius-like transition rate coefficients. The non-dimensional form of the system is given by

$$\frac{dm_i(t)}{dt} = \sum_{(i,j)} e^{-u m_j(t)} m_j(t) - \sum_{(i,j)} e^{-u m_i(t)} m_i(t). \quad (1)$$

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