Study of nonlinear kinetic equation for grain growth

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The motivation for this study is the technological process of sintering. During this process grains of ceramic powders are compacted to a single body without grain liquefaction by exerting heat and/or pressure. Sintering is a complex process in which many physical mechanisms contribute. A common observation in sintering studies is that grains (crystallites) grow either normally, leading to a uniform grain distribution, or abnormally leading to large non-homogeneities in grain size.

We study a nonlinear kinetic model of mass exchange between interacting grains introduced in [1]. The transition rates follow the Arrhenius equation with an activation energy that depends dynamically on the grain masses and an activation parameter. In the two-grain system the activation parameter can be absorbed in the initial conditions for the grain masses, and 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 (normal) and growth-decay (abnormal or reverse diffusion) kinetics. The equilibrium states are determined by the initial conditions, and they are defined by the mass equipartition and mass separation nullcline curves.

Using numerical simulations we show that the grain system maintains the diffusive and growth-decay regimes, even if the transfer rates are perturbed by white noise. However, the presence of the noise can reverse the sign of the equilibrium mass difference leading to the growth of the initially smaller grain at the expense of the larger.

We also investigate a multi-grain chain with nearest-neighbor interactions. Diffusive (normal) and growth-decay (abnormal) regimes are established as well, but the approach to equilibrium is considerably slower than in the case of the two-grain system and includes non-monotonic changes of grain mass. We then add a cellular automaton step to the evolution of the system which enforces the coalescence of neighboring grains if their size ratio exceeds a specified threshold. We study the average grain radius evolution of the modified system as a function of the activation parameter, and we compare the temporal evolution of grain sizes with the Ostwald ripening coarse-graining behavior.

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