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Statistical mechanics of normal grain growth in one dimension: A partial integro-differential equation model

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A B S T R A C T

We develop a statistical-mechanical model of one-dimensional normal grain growth that does not require any drift-velocity parameterization for grain size, such as used in the continuity equation of traditional mean-field theories. The model tracks the population by considering grain sizes in neighbour pairs; the probability of a pair having neighbours of certain sizes is determined by the size-frequency distribution of all pairs. Accordingly, the evolution obeys a partial integro-differential equation (PIDE) over 'grain size versus neighbour grain size' space, so that the grain-size distribution is a projection of the PIDE's solution. This model, which is applicable before as well as after statistically self-similar grain growth has been reached, shows that the traditional continuity equation is invalid outside this state. During statistically self-similar growth, the PIDE correctly predicts the coarsening rate, invariant grain-size distribution and spatial grain size correlations observed in direct simulations. The PIDE is then reducible to the standard continuity equation, and we derive an explicit expression for the drift velocity. It should be possible to formulate similar parameterization-free models of normal grain growth in two and three dimensions.

1. Introduction

Normal grain growth (NGG) refers to the gradual increase of the mean grain or crystal size $\bar{x}$ of a polycrystalline material, as grain-boundary motion causes larger grains to consume smaller grains and small grains to be eliminated. For over five decades, NGG has been studied as a fundamental process affecting texture evolution in metals and geological materials [1,2], and more broadly in connection with coarsening dynamics (e.g. soap-bubble growth) in various physical, social and biological systems; e.g. [3–6]. It is observed that, at large time t, NGG obeys the growth law

$$\bar{x} \sim (Ct)^m \tag{1}$$

(where the grain-growth exponent m and bulk growth rate C are positive constants), with the frequency distribution $n(x, t)$ of the grain size x tending to a statistically quasi-stationary, or 'invariant', self-similar state. For NGG in two- and three-dimensional (2D and 3D) polycrystals with uniform grain boundaries, whose migration rate is curvature-driven, a parabolic growth law with $m = 1/2$ has been established through theoretical considerations [7,8] and numerical simulations (e.g. [9–12]), and finds support also from laboratory experiments [13] (see discussion in Ref. [1]).

Statistical mean-field theories have been instrumental for explaining how such coarsening arises from grain-scale kinetics under the space-filling constraints that grains do not overlap and no voids appear as grain boundaries move. These theories describe the process by regarding each grain as embedded in the mean environment of the population [1]. In the Hillert-Mullins -type "drift models" [14,15], the grain-size distribution n obeys the continuity equation

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x}(vn(x,t)) = 0, \tag{2}$$

where the drift velocity v (= dx/dt) represents grain exchange between different sizes. One would expect that, in a grain system where the rules of grain-boundary migration and associated topological reorganization are all known or prescribed, the evolution can be tracked by a 'complete' statistical-mechanical model based on nothing besides the rules, i.e. not involving extraneous assumptions or approximations informed by the actual outcomes of the NGG dynamics. This means that, if Eq. (2) is a valid model, then a self-contained recipe for the velocity v ought to exist (and hopefully can be found). However, as outlined below, all current models invoke some kind of parameterization for v: thus there is a knowledge gap.

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The purpose of this paper is to provide a mean-field model for NGG in 1D that is complete in the above sense. The model takes the form of a partial integro-differential equation (PIDE), not a partial differential equation. We detail its derivation, explore its relationship with Eq. (2) and compare its predictions to direct simulations of the system. As Mullins [15] explained, Eq. (2) stems from a Fokker-Planck formulation and contains no diffusion term (unlike as envisaged in Louat's model [16]) when the growth process is dominated by curvature-driven grain boundary motion rather than stochastic switching events in grain size or network topology. Our work tackles the same regime.

Hillert's [14] original parameterization for the drift velocity is

$$v = \alpha k\left(\frac{1}{x_c} - \frac{1}{x}\right), \tag{3}$$

where x_c is a time-varying critical grain size ($\propto \bar{x}$), k is the product of grain-boundary energy and mobility, and α is an order-one parameter that varies with the number of spatial dimensions in the system. Eq. (3) summarizes the tendency that grains larger than x_c grow and smaller than x_c shrink; it assigns a single drift velocity to grains of equal size, even though such grains are neighboured by grains of different sizes so they do not grow or shrink at the same rate. By using techniques of the Lifshitz-Slyozov-Wagner [17,18] theory for coarsening dynamics in solid solutions, Hillert predicted long-time parabolic growth with Eqs. (2) and (3) and calculated the corresponding invariant grain-size distribution. However, since his work, shortcomings of the model has spurred many 'modified' mean-field models seeking to improve the parameterization. A first key shortcoming is that Hillert's invariant grain-size distribution mismatches the invariant distributions found in direct 2D and 3D simulations; e.g. [9–11,19,20]. A second issue, exposed also by simulations, is that "spatial grain size correlations" develop as NGG occurs [21–23], with small grains becoming neighboured by more large grains than expected from $n(x, t)$ (which is not surprising because the former grains have lost material to the latter), and large grains neighboured by more small grains than expected from $n(x, t)$ (the former grains have gained material from the latter). This finding conflicts with the idea behind Eq. (3) that different-sized grains evolve under the same environment. Approaches to modify Hillert's drift-velocity parameterization include: (i) pre-multiplying $1/x_c$ in Eq. (3) by an empirically-tuned function $f(x/x_c)$ so that the effective critical grain size x_c/f varies with x to mimic observed neighbour-size correlations [21,22,24]; and (ii) using topological considerations to formulate alternative functions to link v to the reduced grain size $x/\bar{x}$ (e.g. [25–30]). Some of the latter approaches deduce the rate of grain area/volume evolution by accounting for the topological class (number of sides) of the grains (e.g. [30]) and invoke the von Neumann–Mullins 2D growth law [31,32] or its 3D extension [33]. Still other models track the grain-size distributions in different topological classes with separate continuity equations [34,35], although they are not usually considered as being of Hillert-Mullins type. We do not review the large number of modified Hillert theories here but point the reader to the paper by Ref. [36] for further background. Crucially, all modified theories contain adjustable parameters/coefficients that are determined through fitting to the observed dynamics (typically the invariant grain-size distribution). The model derived in this paper has no such necessity.

We see value in investigating a parameterization-free theory. The modified Hillert theories have engendered a tradition of invoking parameterizations to "close" the mean-field description. Such approach is useful because an ansatz posed for the resulting model often yields an analytical solution that can be evaluated straightforwardly for the invariant grain-size distribution. But parameterizations sacrifice physical understanding of the phenomenon, as the basis of some parameters involved remains incompletely known (their values do not derive from first principles), and both the model and its fit to the observed invariant grain-size distribution are ultimately approximate. The choice of parameterization is also not unique; more parameters could mean higher degrees of freedom for empirical fitting, and different parameterizations can predict parabolic growth with near-identical-looking invariant $n(x,t)$. Some modified theories even assume self-similarity for n as a starting condition. As we shall see, our PIDE model has none of these limitations and captures collaborative grain-growth dynamics to a sophisticated level: it predicts the observed neighbour grain-size correlations, similarity scaling, invariant grain-size distribution, and relationship between k and the bulk growth rate C *without parameter tuning*. The PIDE also tracks system evolution outside the self-similar state. It is not analytically solvable by us so far, but this does not mean it is invalid or inappropriate.[1] We are not suggesting that a 'complete' formulation is superior to the Hillert-based approximate models, but rather it is an essential part of our knowledge of NGG. Note that our model treats NGG in *one dimension* only. However, the insights gained from it suggest there is hope for complete mean-field formulations for NGG in 2D and 3D, despite vastly increased topological complexities. We consider this avenue briefly at the end of the paper.

2. Model

2.1. One-dimensional NGG system

Fig. 1a shows our system, in which a large population of linear crystals/grains, whose sizes we denote by x (> 0), participates in NGG. Following previous work [37,21,24] we assume (by analogy to curvature-driven kinetics in 2D/3D) that each grain boundary between adjacent grains migrates into the smaller grain at a speed proportional to the difference between their size reciprocals $1/x$. Thus a grain of size x_0 having left and right neighbours sized x_{1L} and x_{1R} (respectively) grows at the instantaneous rate

$$\dot{x}_0 = k\left[\left(\frac{1}{x_{1R}} - \frac{1}{x_0}\right) - \left(\frac{1}{x_0} - \frac{1}{x_{1L}}\right)\right], \tag{4}$$

where k (constant) has the same meaning as in Eq. (3). A grain vanishes when two grain boundaries merge. Although this analogue system is an idealization as there are no curved grain boundaries in 1D, its reduced geometry—grains always having two sides, the only switching events being grain-boundary merging—aids our goal of seeking analytical understanding. (In this regard, even 2D models of NGG lose some of the topological complexity of NGG in 3D.) Moreover, as found by Refs. [21,24] and confirmed by our direct kinetic simulations (Fig. 1b–e), the 1D system displays the essential properties of NGG behaviour: its grain population coarsens following parabolic growth and attains an invariant self-similar $n(x, t)$ at large time (Fig. 1b–e).

Spatial grain size correlations occur in this 1D system also, as reported by Hunderi and his colleagues [21,24]. These authors put forward a modified Hillert model using Approach (i) described in the Introduction, i.e.

$$v = 2k\left(\frac{f(x/x_c)}{x_c} - \frac{1}{x}\right), \tag{5}$$

[1] Many valid models describing complex phenomena without resorting to parameterizations have not yielded to analytical solution.