Anomalous exponent in the kinetics of grain growth with anisotropic interfacial energy

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The effect of grain-boundary orientational anisotropy on growth kinetics is examined within the context of stochastic theories of grain growth. Grain growth is characterized by power laws of the type, $l \propto t^{\alpha}$, where l is some linear dimension measuring grain size and t is the time. In the case of normal grain growth the growth exponent is 0.5. It is shown that grain-boundary anisotropy leads to a slower growth kinetics with an anomalous exponent of 0.25 in agreement with Q-state Potts models of grain growth. [S0163-1829(97)01202-2]

I. INTRODUCTION

Stochastic theories of grain growth are emerging as useful approaches in treating the phenomenon of grain growth as a geometrically complex dynamic process.[1–6] In some of these models,[3–6] the grain growth process possesses a deterministic drift component and a stochastic component. Grain growth is then described by a Fokker-Planck continuity equation dealing with the grain-size distribution and its evolution in time. In this type of equation, the drift component arises from curvature effects which causes small grains to shrink and large grains to grow.[7] The physical meaning of the diffusionlike random term, however, is not completely established. The stochastic nature of the process may be interpreted on the basis of local statistical variations of environment in the polycrystal since individual grains may evolve differently from the purely deterministic behavior depending on the characteristics of the surrounding grains.[4–6] An alternative interpretation of the random term is put forward in stochastic theories in which the drift term is omitted, that is, theories where grain growth is described as a random walk in grain-size time space.[1,2] There, the stochastic term results from the random motion of grain boundaries and provides the only mechanism for grain growth.

Stochastic theories predictions nonetheless are consistent with experimental observations of normal grain growth. In particular, these theories predict power growth laws where a single length scale l (a linear measure of the growing grains) evolves with time as $l(t) \sim t^{\alpha}$ with $\alpha = 0.5$. Stochastic theories of grain growth can also predict growth exponents smaller than 0.5 provided *ad-hoc* modifications such as time (or grain-size) dependent diffusion coefficients are introduced.[1,2,6]

In this paper we consider the effect of grain-boundary anisotropy on the kinetics of grain growth. For this we treat the case of two-dimensional growth within the context of stochastic theories of grain growth.

In Sec. II, we introduce and solve a discrete one-dimensional stochastic equation with absorbing boundary conditions as grain size decreases to zero. This equation represents normal grain growth with isotropic interfacial energy.

The extension of the stochastic model to modeling grain growth in anisotropic polycrystals is presented in Sec. III. The growth exponent in the anisotropic model is found to take the reduced value of 0.25, in good agreement with computer simulations of Q-state Potts models of growth.[8,9] In keeping with standard nomenclature from diffusion,[10] this slower growth process is called anomalous grain growth in contrast to normal grain growth. Anomalous grain growth described in the present paper, like normal grain growth, involves a collective evolution of all the grains in the microstructure. It is not to be confused with abnormal grain growth (although unfortunately sometimes qualified of anomalous) where a single large grain in a microstructure of comparatively small grains grows by consuming its neighbors.[11,12] Finally, the conclusions drawn from this work as well as future improvements of the model are reported in Sec. IV.

II. ONE-DIMENSIONAL STOCHASTIC MODEL OF ISOTROPIC GRAIN GROWTH

We make the assumption that two-dimensional grain growth can be modeled via a one-dimensional stochastic equation of the form:

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial^2}{\partial x^2}[AP(x,t)], \tag{1}$$

where $P(x,t)$ is a distribution of grains with some linear dimension x at time t. A is a rate factor independent of P. Equation (1) is subjected to the boundary condition that grains are destroyed at $x=0$, that is $P(x=0,t)=0$. In this model, although the evolution of the grain size is stochastic, the microstructure exhibits at a statistical level a more regular and well defined behavior corresponding to a diffusionlike evolution. In a large population of grains, the number of grains with linear dimension between $x-dx/2$ and $x+dx/2$ at time t, is given by $P(x,t)dx$. Any change in this population due to the random evolution of grain size arises from fluxes from neighboring regions of the distribution. The continuity equation (1) assumes that these fluxes depend on the population from which they arise.

Louat,[1] Chen,[2] and Pande[6] claim that studying grain growth in two or three dimensions with a one-dimensional diffusionlike equation is equivalent to monitoring grain size by a linear intercept method. Under this hypothesis, $P(x,t)$, measures the number of grains with linear dimension (as opposed to grain size) x intercepted by a straight line on a micrograph. It should be noted that the intercept length distribution, $P(x,t)$ may not have necessarily the same functional form as of the grain-size distribution in two or three dimensions. To stress this difference, Thorvaldsen[3] considers a thought experiment with a material where growth is driven solely by size difference. The grain-size distribution of a three-dimensional microstructure where all the grains have identical sizes is given by a δ function indicating no growth. In contrast, the intercept method will give a distribution of intercept lengths showing a range of ''grain sizes''[3] which indicates growth. One may argue, however, that repeating the intercept measurement at different times during some annealing period will show no evolution in the intercept length distribution, proving that there is no growth.

Since experimental grain-size measurements are commonly based on the intercept procedure,[13,14] we will focus on the calculation of the mean linear intercept length to provide information on the growth kinetics. In the case of isotropic grain growth where the microstructure is homogeneous, the time evolution of the intercept length distribution will provide unambiguous information on the growth kinetics, and in particular, on how grain linear dimensions (measured by the intercept length) may scale with time during the growth process.

Equation (1) may not represent thoroughly the phenomenon of grain growth as it does not include a drift term, but it will serve as a prototypical equation for investigating the effect of spatial variations in grain-boundary properties on the kinetics laws due to the random term in stochastic theories of grain growth.

Under the assumption that A is independent of x and t, and upon discretization of space, Eq. (1) becomes

$$\frac{dP_n(t)}{dt}=W[P_{n-1}(t)-2P_n(t)+P_{n+1}(t)], \tag{2}$$

where n $(n=0,\pm1,\pm2,\ldots)$ denotes sites on a lattice, $P_n(t)$ is the number of grains with linear dimension equal to na at time t (a being the mesh size in space). $W=A/a^2$, stands for the nearest-neighbor transfer rate taken to be the same on each lattice site.

Laplace transforming (LT) Eq. (2), reduces the differential equation to the simpler form:

$$W\widetilde{P}_{n-1}-(2W+\omega)\widetilde{P}_n+W\widetilde{P}_{n+1}=-P_n(t=0) \tag{3}$$

with

$$\widetilde{P}_n(\omega)=\mathrm{LT}(P_n(t))=\int_0^\infty P_n(t)e^{-\omega t}dt. \tag{4}$$

A more compact form of Eq. (3) is given by

$$\overleftrightarrow{H}_p\cdot\widetilde{\mathbf{P}}=-\mathbf{P}(t=0), \tag{5}$$

where $\overleftrightarrow{H}_p$ is a tridiagonal infinite square matrix and $\mathbf{P}$ is an infinite vector.

The solution to Eq. (5) must be consistent with the initial condition of an arbitrary distribution. We consider the initial condition $P_n(t=0)=\delta_{n,m}$ where δ is the Kronecker symbol. With this condition, Eq. (5) can be written in condensed form as

$$\overleftrightarrow{H}_p\cdot\overleftrightarrow{D}=-\overleftrightarrow{I}, \tag{6}$$

where $\overleftrightarrow{I}$ is the unit matrix.

The preceding equation shows that with a δ initial condition, the Laplace transform of the distribution P is the Green's function $\overleftrightarrow{D}$ associated with the operator $\overleftrightarrow{H}_p$. Using the isomorphism between Eq. (3) and the equation of motion of an infinite harmonic chain,[15] one obtains solutions to Eq. (6) in the form

$$D_{n,m}=-\frac{1}{W}\frac{\tau^{|n-m|+1}}{\tau^2-1}, \tag{7a}$$

where the quantity τ is defined as

$$\tau=\xi-\sqrt{\xi^2-1} \tag{7b}$$

with

$$\xi=1+\frac{\omega}{2W}. \tag{7c}$$

Solution (7) does not satisfy the absorbing boundary condition, $D_{n=0,m}=0$. Such a solution is given by

$$D_{n,m}=-\frac{1}{W}\left(\frac{\tau^{|n-m|+1}}{\tau^2-1}-\frac{\tau^{n+m+1}}{\tau^2-1}\right), \tag{8}$$

where τ has the same definition as in Eq. (7b) and $n,m=0,1,2,\ldots$.

To recover the Green's function as a function of time t we perform an inverse Laplace transform on Eq. (8). After transformation, one obtains the solution of Eq. (6) satisfying the boundary condition $D_{0,m}(t)=0$, and the initial condition $P_n(t=0)=\delta_{n,m}$ in the form

$$D_{n,m}(t)=e^{-2Wt}[I_{|n-m|}(2Wt)-I_{(n+m)}(2Wt)], \tag{9}$$

where I_v is the modified Bessel function of order v.

For convenience, we modify the initial condition to be $P_n(t=0)=N_0\delta_{n,1}$ where N_0 is the total number of grains intercepted by some straight line. The length of that straight line is therefore $L_0=N_0a$. This initial condition may correspond to a microstructure where all the intercept lengths are the same. Although somewhat artificial, this choice will affect the short-time evolution of the distribution of linear dimensions but will not have any influence on the asymptotic long-time limit. The distribution, $P_n(t)$, is obtained as

$$P_n(t)=N_0D_{n,1}(t)=\frac{N_0 2n}{2Wt}e^{-2Wt}I_n(2Wt) \tag{10}$$

for $n=1,2,\ldots$ and $P_0(t)=0$.

To verify that the distribution given by Eq. (10) conserves length, one calculates

$$\overline{L}=\sum_{n=0}^{\infty}naP_n(t)=\frac{N_0 2a}{2Wt}e^{-2Wt}\sum_{n=1}^{\infty}n^2I_n(2Wt). \tag{11}$$

Using the recursive properties of Bessel functions, one shows that Eq. (11) gives $\overline{L}=N_0a$. This is the initial length of the straight line used to measure the intercept length distribution. Summing the distribution, $P_n(t)$, over all the n's gives the total number of grains intercepted by a straight line of length L_0,$N(t)$. It is straightforward to show that

$$N(t)=N_0 e^{-2Wt}[I_0(2Wt)+I_1(2Wt)]. \tag{12}$$

In order to extract a scaling law for linear dimension as a function of time, we first consider the asymptotic behavior of Eq. (12) when $t\to\infty$. For large values of the argument, x, the modified Bessel function $I_n(x)$ behaves asymptotically as $e^x/\sqrt{2\pi x}$, leading to the long-time limit for $N(t)$:

$$N(t)\approx N_0\sqrt{\frac{l}{\pi W}}t^{-1/2}. \tag{13}$$

Since in the case of an isotropic system, the mean intercept length, $l=L_0/N(t)$ represents some linear dimension characteristic of grain size, we conclude that grain size should scale as $l\propto t^{0.5}$. This is the well-known result of parabolic grain growth in isotropic media.

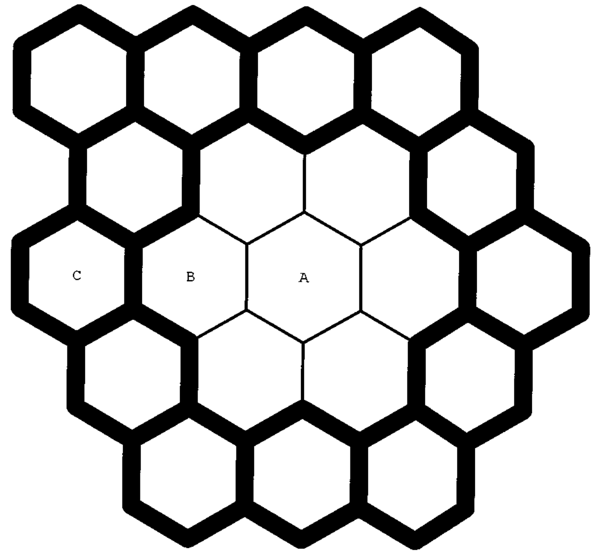

FIG. 1. Schematic representation of a cluster of grains separated by low-angle grain boundaries (thin lines) surrounded by grains forming high-angle grain boundaries (thick lines). For the sake of simplicity we have drawn all the grains as idealized six-sided grains of the same size. The grains B and C possess at least one high-angle grain boundary and belong, therefore to the class $y=0$. The grain labeled A is embedded within the cluster; it belongs to a class $y\neq 0$. The value of y is determined by the distance of A to the closest highly misoriented grain.

III. ANISOTROPIC GRAIN GROWTH

When anisotropy of grain boundaries becomes significant, the physical representation of a polycrystal should deal not only with grain configuration but also with grain orientations. In stochastic theories of isotropic grain growth, variability in spatial configuration of grain boundaries may be accounted for by the random term. The task at hand is to incorporate the effect of a spatial distribution of grain orientation in the statistical model of grain growth. There are theoretical and experimental indications that anisotropic microstructures contain clusters (or extended regions) composed of grains separated by grain boundaries belonging to the same category (i.e., low-angle or special grain boundaries for instance).[16–19] In this paper, we will limit our discussion to a binary classification of grain boundaries: low-angle grain boundaries with low energies and high-angle grain boundaries with high energies. Other classifications such as low-angle, special and high-angle general grain boundaries may be used as well. During the grain growth process, low-energy grain boundaries separating grains of small misorientation will evolve at rates which are small compared to that of high-angle grain boundaries. Clusters of grains separated by low-angle grain boundaries will survive until some neighboring grain with a different crystallographic orientation grows to that size.[8] The survival of clusters of small grains will lead to broader grain-size distributions and a slower grain growth kinetics.[8]

To account for the spatial variability in grain orientation, we introduce an additional degree of freedom or state variable y, in the form of the distance between some grain of interest and the nearest grain with high-angle misorientation with respect to the former. This additional degree of freedom supplements the grain linear dimension (intercept length) x used in the isotropic case. We can now divide the grains into classes, (x,y), of grains with linear dimension x and with the nearest highly misoriented grain at a distance y (see Fig. 1). Let $P(x,y,t)$ be the number of grains in class (x,y) at time t. With this, $P(x,y=0,t)$ represents the number of grains at time t with intercept length x sharing a high-angle grain boundary with some neighboring grain. Only those grains delimited by at least one high-angle grain boundary are susceptible to grow or to shrink. A grain belonging to a class $(x,y\neq 0)$, cannot change in size as it is embedded within some cluster of grains separated by low-angle grain boundaries. To grow or shrink, it has to enter the class $(x,y=0)$. For this it may start at (x,y) with y decreasing over time because of some highly misoriented grain in the microstructure growing and absorbing its neighbors. As the boundary of the growing grain approaches, the grain of interest becomes susceptible of evolution toward the class $y=0$. For grains to change classes, there exist possible physical mechanisms involving topological changes.[20] These topological changes may include vanishing of a neighboring grain or boundary switching which may lead to a modification of the surrounding such that the grain of interest now shares a high-angle grain boundary with some other grain.

Within the context of a stochastic model of grain growth, we write

$$\frac{\partial P(x,y=0,t)}{\partial t}=A\frac{\partial^2 P(x,y=0,t)}{\partial x^2}. \tag{14}$$

This equation is equivalent to Eq. (1) but its action is limited to grains in the class $(x,y=0)$. Since evolution in the degree of freedom y results from grain growth of some other highly misoriented grain, we argue that this evolution is controlled by normal grain growth, that is, it is stochastic with the same rate factor A. We propose the equation

$$\frac{\partial P(x,y,t)}{\partial t}=A\frac{\partial^2 P(x,y,t)}{\partial y^2}. \tag{15}$$

Equations (14) and (15) constitute the basis for a stochastic model of anisotropic grain growth. Upon discretization, these equations become

$$\frac{dP_n(t)}{dt}=W[P_{n-1}(t)-2P_n(t)+P_{n+1}(t)] + W^*[P_{n,1}(t)-P_n(t)] \quad (16)$$

and

$$\frac{dP_{n,n'}(t)}{dt}=W[P_{n,n'-1}(t)-2P_{n,n'}(t)+P_{n,n'+1}(t)], \quad \text{if } n'\geqslant 2 \quad (17)$$

$$\frac{dP_{n,n'}(t)}{dt}=W^*[P_n(t)-P_{n,n'}(t)] - W[P_{n,n'}(t)-P_{n,n'+1}(t)], \quad \text{if } n'=1.$$

Here, $P_n(t)$ and $P_{n,n'}(t)$ stand for the discretized forms of $P(x,y=0,t)$ and $P(x,y,t)$, respectively. The discrete variables n and n' substitute for the continuous variables x and y. The discretization is done with the same mesh size a as in Sec. II, this for the two variables x and y, as they both have unit of length. We have inserted into Eqs. (16) and (17), fluxes with a transfer rate W^* to ensure the continuity condition:

$$\lim_{y\to 0} P(x,y,t)=P(x,y=0,t). \quad (18)$$

These fluxes may be related to the mechanisms which allow passage from one grain class to another as, for instance, topological changes. In general, the transfer rate for these mechanisms does not bear any resemblance to the transfer rate for grain growth. However, since the main objective of this section is to extract an asymptotic kinetics law for anisotropic grain growth, the relative magnitude of W^* compared to W is unimportant, as it is spatially limited to regions in phase space where $y\to 0$. We therefore simplify the set of Eqs. (16) and (17) by choosing $W^*=W$. Under this condition the discretized stochastic equations reduce to

$$\frac{dP_n(t)}{dt}=W[P_{n-1}(t)-2P_n(t)+P_{n+1}(t)] + W[P_{n,1}(t)-P_n(t)] \quad (19)$$

and

$$\frac{dP_{n,n'}(t)}{dt}=W[P_{n,n'-1}(t)-2P_{n,n'}(t)+P_{n,n'+1}(t)] + \delta_{n',1}W[P_n(t)-P_{n,n'-1}(t)]. \quad (20)$$

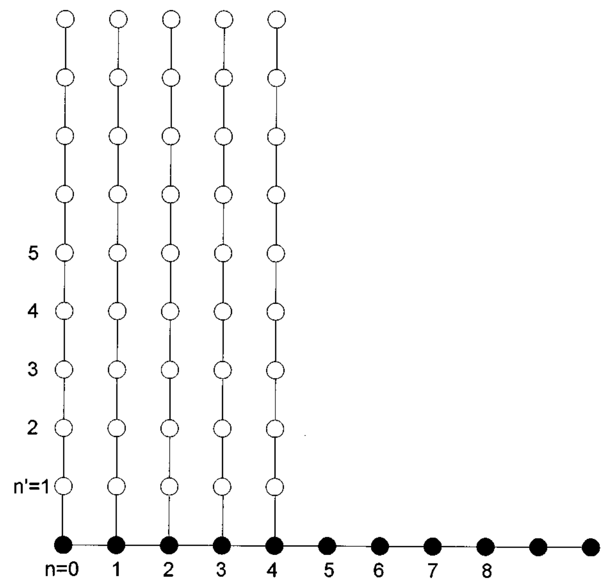

FIG. 2. Discrete phase space for anisotropic grain growth. The horizontal semi-infinite line is called the backbone ($n=0,1,2,\dots\infty$). The vertical semi-infinite lines are the side branches ($n'=1,2,3,\dots\infty$). This space contains an absorbing boundary condition at $n=0$.

This set of equations models a random walk on a two-dimensional phase space constructed by attaching to every site in a one-dimensional discrete space of grain's intercept length (called thereon the backbone) a discrete side branch of distances between highly misoriented grains. It is important to note that the side branches are not linked to each other because grains in a class (n,n') cannot grow to a class $(n+1,n')$. Growth is only allowed along the backbone.

In Fig. 2, we illustrate the discrete phase space used as basis for modeling grain growth with anisotropy. Positions along the backbone are labeled with unprimed indices. These unprimed indices will also be used to label every side branch. Positions along the side branch are referenced with a primed index varying between 1 and ∞. It is now our objective to find the distributions, $P_n(t)$ and $P_{n,n'}(t)$, in the complex networked space of Fig. 2. Similarly to Sec. II, we Laplace transform Eqs. (19) and (20) and seek solutions in the form of the Green's function $\overleftrightarrow{d}$ in the networked phase space of Fig. 2. For this we employ the methods of the interface response theory,[21,22] which allows the construction of the Green's function of a composite system in terms of the Green's functions of its constitutive elements. The mathematical procedure we follow thereon begins with the construction of the Green's function of an infinite linear lattice. This lattice is divided in periodic unit cells of length a and the Green's function is expressed in Fourier space. A semi-infinite linear lattice (side branch) is then grafted onto a unit cell to obtain the Fourier transform of the distribution of an infinite backbone lattice with side branches coupled at every site along the backbone. An absorbing boundary condition at site 0 along the backbone is then imposed on the inverse Fourier transform of that latter function. This mathematical procedure leads to the real-space Green's functions satisfying the absorbing boundary condition at $n=0$:

$$d_{n,m}=-\frac{1}{W}\left(\frac{\tau'^{|n-m|+1}}{\tau'^2-1}-\frac{\tau'^{n+m+1}}{\tau'^2-1}\right), \tag{21a}$$

$$d_{n,m,n'}=-\frac{\tau^{n'}}{W}\left(\frac{\tau'^{|n-m|+1}}{\tau'^2-1}-\frac{\tau'^{n+m+1}}{\tau'^2-1}\right), \tag{21b}$$

where τ has the same definition as before and τ' is given by $\tau'=\xi'-\sqrt{\xi'^2-1}$ with $\xi'=\xi-(\tau-1)/2$. It is worthy pointing out again that the indices n and m stand for sites on the infinite backbone and that the primed index n' relates to a site in the side branch attached to the backbone at site n.

Let us now impose the initial condition of a δ distribution at $m=1$ with N_0 intercepted grains. Under this initial condition, the Laplace transform of the distributions, P_n and $P_{n,n'}$, are expressed as

$$\tilde{P}_n=d_{n,1}, \qquad \tilde{P}_{n,n'}=d_{n,1,n'}. \tag{22}$$

We can now calculate the Laplace transform of the total linear dimension $\tilde{\tilde{L}}(\omega)$ from

$$\tilde{\tilde{L}}=N_0\left\{\sum_{n=0}^{\infty}\sum_{n'=1}^{\infty} na\tilde{P}_{n,n'}+\sum_{n=0}^{\infty} na\tilde{P}_n\right\}. \tag{23}$$

In contrast to Sec. II, the summations are taken over the entire networked space. After insertion of Eqs. (21a) and (21b), Eq. (23) becomes

$$\tilde{\tilde{L}}=\frac{N_0}{W}\left\{\sum_{n=0}^{\infty} na\tau'^n\sum_{n'=1}^{\infty}\tau^{n'}+\sum_{n=0}^{\infty} na\tau'^n\right\}. \tag{24}$$

Since τ and τ' are smaller than one, the different sums in Eq. (23) converge and the total length of all grains intercepted simplifies to

$$\tilde{\tilde{L}}=\frac{N_0 a}{W}\frac{\tau'}{(1-\tau')^2}\frac{1}{1-\tau}. \tag{25}$$

With the help of general Abelian and Tauberian theorems,[23] the asymptotic behavior of $\underline{L}(t)$ for time, $t\to\infty$ can be determined from the asymptotic behavior of $\tilde{\tilde{L}}(\omega)$ for $\omega\to 0$.

For small frequencies, τ and τ' can be approximated by

$$\tau\to 1-\sqrt{\frac{\omega}{W}}, \tag{26a}$$

$$\tau'\to 1-\left(\frac{\omega}{W}\right)^{1/4}, \tag{26b}$$

leading to

$$\tilde{\tilde{L}}\to N_0 a\frac{1}{\omega}. \tag{27}$$

The inverse Laplace transform of Eq. (27) is independent of time, showing that the total length of the intercepting straight line used to measure the intercept length distribution is conversed by Eqs. (21a) and (21b).

We now determine the total number of grains, $\tilde{N}(\omega)$ within the straight line length. It is calculated by summing Eqs. (21a) and (21b) over the backbone and the side branches. We write

$$\tilde{N}=N_0\left\{\sum_{n=1}^{\infty}\sum_{n'=1}^{\infty}\tilde{P}_{n,n'}+\sum_{n=1}^{\infty}\tilde{P}_n\right\}=\frac{N_0}{W}\sum_{n=1}^{\infty}\tau'^n\left\{\sum_{n'=1}^{\infty}\tau^{n'}+1\right\}. \tag{28}$$

Calculating the sums explicitly, one finds

$$\tilde{N}=\frac{N_0}{W}\frac{1}{1-\tau}\frac{\tau'}{1-\tau'}. \tag{29}$$

The asymptotic behavior of $\tilde{N}(\omega)$ when $\omega\to 0$ is

$$\tilde{N}\to N_0 W^{-1/4}\omega^{-3/4}, \tag{30}$$

which inverse Laplace transform gives

$$N(t)\to N_0(Wt)^{-1/4} \quad \text{when} \quad t\to\infty. \tag{31}$$

This result can be compared directly against the isotropic case indicating a slower growth when anisotropy in grain-boundary energy due to grain misorientation is accounted for. A question regarding the estimation of the growth law in terms of grain size arises. We have seen that the microstructure becomes less homogeneous as one introduces grain-boundary anisotropy. The microstructure may be considered to consist of extended regions of small grains (clusters) separated by low-angle grain boundaries and of larger grains bounded by high-angle grain boundaries. It has been shown,[8] however, that the grain-size distribution for anisotropic growth is time invariant if the grain size is scaled by the mean grain size. This observation suggests that the mean grain size, even for the less homogeneous anisotropic microstructure, is a valid scaling parameter. In consequence, one may employ the intercept method and the mean grain linear dimension as a measure of grain size to provide information on the growth kinetics. In addition, in order for the mean intercept length, $l=\bar{L}/N(t)$, to give statistically significant results on the grain size, one needs to employ an intercept which length is larger than the correlation length of the microstructure. At this larger scale, the intercept procedure gives a satisfactory statistical measure of the mean grain linear dimension.

Provided that $\bar{L}$ is sufficiently large, we find in the case of anisotropic grain growth that grain size as measured by the linear dimension l scales asymptotically as

$$l \propto t^{1/4}. \tag{32}$$

Equation (32) is the main result of this paper. It states that grain growth kinetics is slowed down by anisotropy with an anomalous growth exponent equal to 1/4.

The same anomalously low value of the growth exponent has also been found in the dynamics of grain growth[8] and ordering process[9] in Q-state Potts models. These computer simulations are two-dimensional Monte-Carlo simulations with anisotropic grain-boundary energies. In the work of Grest, Srolovitz, and Anderson,[8] the growth exponent is shown to decrease with increasing degree of anisotropy to a limiting value of 0.25. The growth exponent of 0.25 is observed for several forms of the interfacial energy/misorientation angle function indicating some universality.

It is worthy noting that the grain-size distribution function from the computer simulation of normal grain growth with a Q-state Potts model[24] seems to be quite well represented by a distribution proposed by Louat.[1] More remarkably, the distribution of grain radii data determined from a cross-sectional area of three-dimensional Q-state Potts model of normal grain growth[25] is best described by a generalization of Louat's distribution function. These observations suggest a close resemblance in the underlying principles of stochastic and Q-state Potts models of growth. The agreement in the value of the growth exponent of our stochastic model of anisotropic growth and the Monte Carlo calculations of Grest, Srolovitz, and Anderson[8] supports this assertion even further.

IV. CONCLUSIONS

We have presented the derivation of asymptotic kinetics laws within the context of stochastic theories of grain growth. For mathematical reasons we have limited ourselves to the investigation of the effect of grain-boundary anisotropy on grain growth modeled with a prototype one-dimensional continuity growth equation for the distribution of grain linear dimensions measured with the intercept method. This equation consists of a random term only. Although this equation does not include grain-boundary curvature effects, it may serve as a means to quantify the difference in kinetics between isotropic and anisotropic grain growth. Grain growth with isotropic grain-boundary energies is studied through the time evolution of the distribution of grain linear dimensions (intercept length) in a one-dimensional homogeneous space. We argue that grain growth with anisotropic grain-boundary energies should take place on a two-dimensional networked space composed of one-dimensional side branches attached along a one-dimensional backbone. The side branches correspond to a new degree of freedom characterizing the distance between highly misoriented grains and controlling the evolution of grains. All the derived solutions for the grain distributions obey an absorbing boundary condition at zero size and conserve overall length. In the case of anisotropy we have found that grain size, as measured by the intercept length, increases as time at the power 0.25. This anomalous grain growth kinetics of our stochastic model is in excellent agreement with Monte Carlo simulation of Q-state Potts models of growth[8,9] suggesting close similarities between these two models.

The growth exponent of 0.25 calculated in the present paper is obtained with semi-infinite side branches. These semi-infinite side branches model a system for which the minimum distance between highly misoriented grains does not have an upper bound. However, one may consider the case of microstructures constituted of clusters of grains with small misorientation possessing a bounded size. For a cluster with a bounded size, the distance between grains with high misorientation is limited to some length on the order of the mean cluster size. A stochastic model of grain growth in an anisotropic polycrystal may then be constructed with a phase space composed of finite-length side branches grafted onto a backbone. One may treat two limiting cases with finite length side branches. Following the procedure established in Sec. III, we have calculated the growth exponent for a system where the side branches possess the same constant finite length. In that case the two-dimensional discrete lattice possesses periodicity along the backbone and we find that grain growth is normal with a growth exponent of 0.5. The length of the side branches causing delays in the growth should not be constant but should more realistically increase along the backbone as the cluster size is expected to scale with the mean grain size.[8] We have not been able yet to solve the stochastic growth equation in that two-dimensional nonperiodic phase space. However, the fact that the mean length of the side branches in that latter lattice is infinite (and not finite as for the former) suggests that grain growth in that case will also be anomalous.

The question of what happens to the anisotropic growth exponent when the grain growth process possesses a deterministic curvature-driven drift component and a stochastic component remains partially unanswered. Experiments show that curvature effects are important for small grains and that larger grains grow in a more random fashion.[26] In the case of isotropic growth, consideration of both components give the growth exponent of 0.5.[6] In anisotropic microstructures, at fixed curvature, the deterministic driving force for growth should vary from grain boundary to grain boundary as the interfacial energy depends on grain misorientation. At fixed misorientation, the driving force is inversely proportional to the grain-boundary curvature. It is worth noting that our networked model of anisotropic growth includes an implicit reference to anisotropy in the deterministic curvature-driven force in the form of the binary classification of grain boundaries in terms of low-energy (small-angle) and high-energy (high-angle) grain boundaries. The construction of a phase space composed of side branches attached to a backbone reflects only implicitly a spatial and a grain size variability in grain-boundary driving force. A more explicit account of a deterministic drift term, perhaps by solving for the Green's function of the Fokker-Planck growth equation in a continuous two-dimensional networked space with side branches or by applying some curvature driven external potential onto our discrete networked space, will be the subject of a future study.

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