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Kinetics of transformation with nucleation and growth mechanism: Two- and three-dimensional models

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Theoretical results on the kinetics of transformations with nucleation and growth mechanisms in homogeneous systems during isothermal annealing are reported. The present derivations start from a probability calculation in a finite discrete assembly. In the simplest case with a constant growth rate the results of the formulation agree with the classical Avrami equation for two- and three-dimensional systems. Furthermore, by calculating the survival probability step by step for separate occurrences, the relationships between interfering processes and the effects of neighboring nuclei are revealed. In particular, the distribution of nuclei pairs with distance is determined. Various cases of preferred nucleation in specialized regions, such as linear zones (e.g., dislocations), planar areas (e.g., grain boundaries), or three-dimensional partial volumes, are analytically solved and these solutions can be directly used for the interpretation and evaluation of experimental measurements. © *1996 American Institute of Physics.* [S0021-8979(96)01606-2]

I. INTRODUCTION

In the preceding article by the present authors, a new method for analytically studying the kinetics of the phase transformation with nucleation and growth mechanisms has been introduced.[1] In contrast to the classical theory,[2–5] such as the well-known Avrami equation, the new derivation is based on probability calculation in a finite and discrete system and thus follows direct logic. The treatment of a one-dimensional (1D) system in the preceding article[1] has yielded not only a kinetics equation which agrees with the Avrami equation in the simplest case, but also functions describing the distribution of the grain pairs.

In this work, the study is extended to the general two- and three-dimensional (2D and 3D) cases by maintaining the basic assumption that each lattice site is indistinguishable which means that both nucleation rate and growth rate are not functions of space. Because many surface problems can be viewed as grain boundary nucleation and growth in two dimensions, investigation of the transformation behavior in 2D systems is of practical interest.

In the classical treatment enormous difficulties arise from the study of problems such as the superposition of many parallel progressing processes and the effects of neighboring nuclei. These can be solved by the present method which is based on calculating the probability of separate occurrences. Preferred nucleation may be realistic in different kinds of transformations. Special conditions for nucleation and growth are considered in this work by studying the nucleation at line defect, at planar boundary, and in the restricted volume, which yields information about the transition from heterogeneous to homogeneous nucleation.

II. TRANSFORMATION WITH HOMOGENEOUS NUCLEATION

A. Two-dimensional model

In the present work as in the preceding article,[1] the general kinetics of the transformation is investigated by considering that both the nucleation rate and the growth rate are known as functions of the relevant parameters. The nucleation rate I is defined in the conventional sense, namely $I\Delta V\Delta t$ means the number of stable nuclei which are capable of growing formed in the volume ΔV during the time interval Δt. For the infinitesimal ΔV and Δt the number of nuclei is to be understood as the probability of forming a nucleus in volume ΔV and time Δt. Also in the present treatment we consider only the simple case with the nucleation rate I independent of the space and a constant growth rate λ for any growing nucleus.

Starting from the finite and discrete approach, we divide the transformation process into steps by choosing Δt as the time interval for each step. Then we divide the whole two-dimensional model lattice with size $L\times L$ into $M\times M$ sites and set the distance interval $\Delta x=\Delta y=\lambda\Delta t=L/M$. Since with these definitions each site has a volume of $\Delta x\Delta y$, the probability for an untransformed site to form a nucleus during time interval Δt at time t or at the nth step is obtained

$$p_n=I_n\Delta t\Delta x\Delta y=\frac{I_nL^3}{\lambda M^3}. \tag{1}$$

The nucleation rate and the growth rate λ are considered to be independent, but the quantity p_n depends not only on the nucleation rate, but also on the selection of ΔV and Δt, so that in this formulation the growth rate λ is also included. We consider the nucleation rate as a function of the step number n, so we rewrite I as I_n and in this case p_n varies

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with the step number n. The probability for the site considered not to form a nucleus during all n steps is yielded by

$$q_n=\prod_{i=1}^{n}(1-p_i). \tag{2}$$

The probability that the considered site will not be captured by the growth of its sth neighbor up to the nth step is equal to the probability that this sth neighboring site has not experienced nucleation up to the $n-s$ step. For calculating the total survival probability for the considered site, the influence of all its neighboring sites has to be taken care of, by counting all sites in each neighboring shell. The survival probability not to be transformed up to the nth step is then obtained as follows:

$$Q=q_n\prod_{i=1}^{n-1}q_{n-i}^{Z_i}, \tag{3}$$

where Z_s is the total number of all sites in the sth neighboring shell. For further derivation we have to assume $p_i \ll 1$ and then we get

$$Q=\exp\left(-\sum_{i=1}^{n}Z_i\sum_{j=1}^{n-i}p_j\right). \tag{4}$$

To calculate the number of sth neighbors we have to use the continuous medium approach by considering that the sth neighboring shell has a radius of $r_s=sL/M$, which yields

$$Z_s=2\pi r_s M/L=2\pi s.$$

Inserting into Eq. (4) and going to the continium limit leads to

$$Q=\exp\left[-2\pi\lambda^2\int_0^t\tau\int_0^{t-\tau}I du d\tau\right]$$

$$=\exp\left[-\pi\lambda^2\int_0^t I(t-\tau)^2 d\tau\right] \tag{5}$$

here the operation

$$\int_0^z x\int_0^{z-x}f(y)dydx=\int_0^z f(y)\int_0^{z-y}xdxdy$$

is used.

If the nucleation rate I is not a function of the annealing time we immediately have

$$Q=\exp\left(-\frac{\pi}{3}I\lambda^2 t^3\right) \tag{6}$$

and for the transformed fraction

$$X=1-Q=1-\exp\left(-\frac{\pi}{3}I\lambda^2 t^3\right), \tag{7}$$

which is identical to the result of the derivation by Avrami.

B. Three-dimensional model

In analogy we divide the whole three-dimensional model lattice into $M\times M\times M$ sites and set the distance interval $\Delta x=\Delta y=\Delta z=\lambda\Delta t=L/M$. Compared to Eq. (1), $\Delta V=\Delta x\Delta y\Delta z$ is yielded, so that we immediately get the probability for an untransformed site to form a nucleus during time interval Δt at time t,

$$p_n=I_n\Delta t\Delta x\Delta y\Delta z=\frac{I_n L^4}{\lambda M^4}. \tag{8}$$

Due to the same considerations as in the derivation of the 2D case, Eqs. (2)–(4) can also be derived for 3D cases, if the corresponding Z_s is substituted. The sth neighboring shell is now the surface of the sphere rather than the perimeter of the circle in the 2D case so that we obtain

$$Z_\tau=4\pi r_s^2 M^2/L^2=4\pi s^2. \tag{9}$$

Inserting this into Eq. (4) yields the following survival probability:

$$Q=\exp\left(-4\pi\lambda^3\int_0^t\tau^2\int_0^{t-\tau}I du d\tau\right)$$

$$=\exp\left(-\frac{4\pi}{3}\lambda^3\int_0^t I(t-\tau)^3 d\tau\right). \tag{10}$$

For a constant nucleation rate I this leads immediately to $Q=\exp(-\pi/3I\lambda^3 t^4)$ and for the transformed fraction

$$X=1-Q=1-\exp(-\pi/3I\lambda^3 t^4), \tag{11}$$

which demonstrates that the Avrami equation for 3D is reestablished.

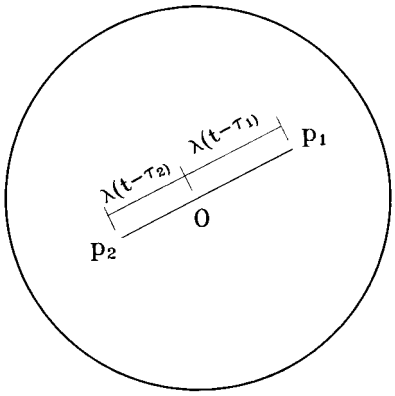

FIG. 1. Impingement of two nuclei at time t, which formed in sites p_1, p_2 and at time τ_1, τ_2, respectively.

C. Distribution of nuclei pairs

As in the preceding article[1] the distribution of pairs with a separating distance y can be determined for 2D and 3D cases. We consider, that at any time t, two growing nuclei meet at the site O, as demonstrated in Fig. 1. The probability, that the site O is not transformed before the impingement is $\exp(-\pi/3I\lambda^D t^{D+1})$ for $D=2$ or 3 denoting the degree of the dimension. If one nucleus forms at τ_1 in the site p_1 and another at τ_2 in the site p_2, the distance between the two nuclei is $y=(2t-\tau_1-\tau_2)\lambda$. For any given site O and the known t and y, p_1 (or p_2) can be selected as all sites within the circle in Fig. 1, so that there are totally $\pi r^2 M^2/L^2$ possible values for the pair p_1 and p_2 in the 2D case. For the 3D case the number of the possible pairs is $4\pi r^3 M^3/(3L^3)$. It is

determined that $r=0$ for $\lambda t<y/2$, $r=(2\lambda t-y)$ in the range of $y/2<\lambda t<y$, and $r=y$ for $t\geqslant y/\lambda$, respectively. By considering impingement at all sites, the probability for impingement of two nuclei with distance y at time t is obtained for the 2D case as

$$P=\frac{\pi r^2M^4}{L^2}\left(\frac{IL^3}{\lambda M^3}\right)^2\exp\left(-\frac{\pi}{3}I\lambda^2t^3\right)$$
$$=\frac{\pi r^2I^2L^2}{\lambda}\exp\left(-\frac{\pi}{3}I\lambda^2t^3\right)\Delta y\Delta t \tag{12a}$$

while for 3D it gives

$$P=\frac{4\pi r^3M^6}{3L^3}\left(\frac{IL^4}{\lambda M^4}\right)^2\exp\left(-\frac{\pi}{3}I\lambda^3t^4\right)$$
$$=\frac{4\pi r^3I^2L^3}{3\lambda}\exp\left(-\frac{\pi}{3}I\lambda^3t^4\right)\Delta y\Delta t. \tag{12b}$$

The integration over time t yields the distribution of nuclei pair with the separating distance. If we define $\omega(y)$ as the fraction of all pairs with a spacing not larger than y, we have for the 2D case

$$f_y=\frac{d\omega}{dy}=\frac{3IL^2}{A_2\lambda}\chi_2\left[\left(\frac{\pi I}{3\lambda}\right)^{1/3}y\right] \tag{13a}$$

and for the 3D case

$$f_y=\frac{4IL^3}{A_3\lambda}\chi_3\left[\left(\frac{\pi I}{3\lambda}\right)^{1/4}y\right]. \tag{13b}$$

The function $\chi_D(\eta)$ is defined as

$$\chi_D(\eta)=C_D\left[\eta^D\int_\eta^\infty\exp(-u^{D+1})du + \int_{\eta/2}^{\eta}(2u-\eta)\exp(-u^{D+1})du\right] \tag{14}$$

for $D=1$, 2, or 3 corresponding to the 1D, 2D, or 3D case. A_2, A_3, and C_D are constants inserted to satisfy the condition

$$\int_0^\infty f_y dy=1,\quad \int_0^\infty\chi_D(\eta)d\eta=1.$$

The dependence of $\chi_D(\eta)$ on the degree of dimension and the reduced distance η is illustrated in Fig. 2.

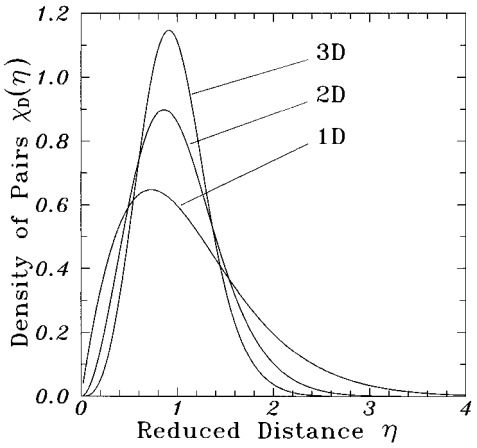

FIG. 2. Distribution of nuclei pairs with the separation distance, calculated by using Eq. (14).

D. Superposition of more than one process

We consider the first case where two nucleation and growth processes take place in parallel. For the sake of illustration we take the 1D lattice as an example.

In each arbitrarily small time interval Δt and in the distance Δx the probability of forming a nucleus of type A is $I_1\Delta t\Delta x$ and forming a nucleus of type B is $I_2\Delta t\Delta x$. During the elapsed time t, following the previously described procedures of our derivation, $\lambda_1 t/\Delta x$ steps have been covered, in process A, while the step number is $t_2/\Delta x$ for process B. The separate probability for each site not to form a nucleus of type A or B up to time t is $q_1=(1-I_1\Delta t\Delta x)^{\lambda_1 t/\Delta x}$ and $q_2=(1-I_2\Delta t\Delta x)^{\lambda_2 t/\Delta x}$, respectively. A site remains untransformed if it is neither captured by a grain of type A nor by one of type B, so that the survival probability is obtained as

$$Q=\prod_{i=1}^{\lambda_1 t/\Delta x}(1-I_1\Delta t\Delta x)^{2(\lambda_1 t/\Delta x-i)} \times\prod_{j=1}^{\lambda_2 t/\Delta x}(1-I_2\Delta t\Delta x)^{2(\lambda_2 t/\Delta x-j)}$$
$$=\exp\left(-2\int_0^t(t-\tau)(I_1\lambda_1+I_2\lambda_2)d t\right). \tag{15a}$$

We can further show that for the 2D case

$$Q=\exp\left(-\pi\int_0^t(t-\tau)^2(I_1\lambda_1^2+I_2\lambda_2^2)dt\right) \tag{15b}$$

and for the 3D case

$$Q=\exp\left(-\frac{4\pi}{3}\int_0^t(t-\tau)^3(I_1\lambda_1^3+I_2\lambda_2^3)dt\right). \tag{15c}$$

It is recognized that instead of the product $I\lambda^D$ for the single process treated in the preceding work, we have $(I_1\lambda_1^D+I_2\lambda_2^D)$ for the two superposing processes with D being the degree of the dimension. This means that the kinetics itself remains in its characteristic form for the superposition of two processes.

For a definite single process the total number of nuclei can easily be calculated by $N=V\int_0^\infty IQdt$, which yields

$$N/V=\left(\frac{3I^2}{\pi\lambda^2}\right)^{1/3}\int_0^\infty e^{-u^3}du\quad\text{for 2D;}$$

$$N/V=\left(\frac{3I^3}{\pi\lambda^3}\right)^{1/4}\int_0^\infty e^{-u^4}du\quad\text{for 3D}$$

with V having the ordinary meaning of the total volume. For two superposed processes, the number of grains of each type can be determined by $N_i/V=\int_0^\infty I_iQdt$, so that we have, e.g., for the 3D case,

$$\frac{N_i}{V}=(\pi(I_1\lambda_1^3+I_2\lambda_2^3)/3)^{-1/4}I_i\int_0^\infty e^{-u^4}du. \tag{16}$$

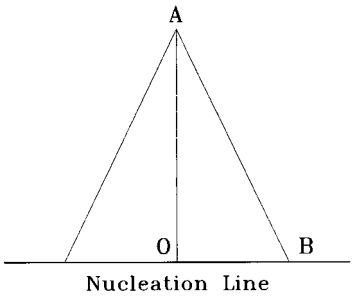

FIG. 3. Growth of grains nucleated at line defect with a constant rate.

We now consider the case for two processes which occur one after another. For example, in the early stage of annealing ($t<t_c$) the single process with nucleation rate I_1 and growth rate λ_1 dominates and after t_c, a second process with I_2 and λ_2 starts. The fundamental equation in the form of integration

$$Q=\exp\left(-\int_0^t (t-\tau) f(I_1,\lambda_1,I_2,\lambda_2)\,dt\right)$$

directly leads to

$$\begin{aligned} &Q=\exp(-I_1\lambda_1 t^2) \quad \text{for } t<t_c, \\ &Q=\exp(I_2\lambda_2 t_c^2)\exp(-(I_1\lambda_1+I_2\lambda_2)t^2) \quad \text{for } t>t_c \end{aligned} \tag{17}$$

for 1D cases. Similar relationships can be obtained for the 2D and 3D cases.

III. KINETICS WITH NUCLEATION IN SPECIAL REGIONS

A. Nucleation at line defects

We consider that the transformation in a lattice can progress by nucleation only along a single line, which corresponds to a dislocation or the edge formed by the intersection of three grains in reality. As shown in Fig. 3, a given site A has a distance $OA=y$ to the nucleation line and $(x^2+y^2)^{1/2}$ to any site B in the line with $OB=x$. The condition for site A not to be captured by a grain nucleated at site B during t is that the site B does not form a nucleus up to the time $t-(x^2+y^2)^{1/2}/\lambda$. The total probability that site A is not captured by a nuclei formed at the considered line is thus obtained,

$$R=q_{k_0}\prod_{i=1}^{m} q_{k_i}^2 \tag{18}$$

the following equation is yielded:

$$k_i=\left[\lambda t-\left(\left(\frac{iL}{M}\right)^2+y^2\right)^{1/2}\right]\frac{M}{L}, \quad m=\frac{M}{L}(\lambda^2 t^2-y^2)^{1/2}. \tag{18a}$$

For $M\to\infty$ we have

$$\begin{aligned} R&=\exp\left\{-2\int_0^{(\lambda^2t^2-y^2)^{1/2}}[\lambda t-(x^2+y^2)^{1/2}]\frac{I}{\lambda}\,dx\right\} \\ &=\exp\left[-I\lambda t^2 f\left(\frac{y}{\lambda t}\right)\right], \end{aligned} \tag{19}$$

where $f(u)=(1-u^2)^{1/2}-u^2\ln[(1+(1-u^2)^{1/2})/u]$. $R(t,y)$ thus means that the probability for a special site having a distance y to the nucleation line is considered not to be captured by nuclei initially formed at the line. For the presence of more than one nucleation line, the superposition can be considered according to the principle studied in Sec. II C. In analogy, if the existence of the nucleation line is determined by a probability p, the real probability to be untransformed is $R'_{\text{real}}=R^p$.

Based on these considerations, we can evaluate a mean survival probability over all sites, if the distribution of the nucleation lines is known. For the case where all lines situate randomly in the lattice, the probability for each column being the nucleation line is thus K/M for the 2D case and K/M^2 for the 3D case, if there are totally K nucleation lines. This implies, that for each site, all columns from 0 to λt can act as the nucleation line with a certain probability. The probability for a site to remain untransformed thus follows:

$$\begin{aligned} Q&=\prod_{i=1}^{\lambda tM/L} R^{KZ_i/M}(t,y=iL/M) \\ &=\exp\left(\frac{2K}{L}\int_0^{\lambda t} Z'_y \ln R(t,y)\,dy\right), \end{aligned} \tag{20}$$

where $Z_s=2$ for 2D growth and $Z_s=2\pi s$ for the 3D case.

Inserting Eq. (19) into this yields

$$Q=\exp\left[-\frac{2KI\lambda^2t^3}{L}\int_0^1 f(u)\,du\right]=\exp\left(-\frac{\pi KI\lambda^2t^3}{3L}\right) \tag{21a}$$

for the 2D case and

$$\begin{aligned} Q&=\exp\left[-\frac{2\pi KI\lambda^3t^4}{L^2}\int_0^1 uf(u)\,du\right] \\ &=\exp\left(-\frac{\pi KI\lambda^3t^4}{3L^2}\right) \end{aligned} \tag{21b}$$

for the 3D case. If we set $I'=KI/L$ and $I''=KI/L^2$ we immediately have $Q=\exp(-\pi/3I'\lambda^2t^3)$ for the 2D case and $Q=\exp(-\pi/3I''\lambda^3t^4)$ for the 3D cases, so that the same results as in Eqs. (6) and (10) are obtained. This indicates that for randomly distributed line defects such as nucleation source the kinetics remains unchanged.

In reality, strong distribution of linear nucleation sources may be expected. As the extreme case, we consider that the nucleation lines are parallel and arranged in a lattice with a separation distance l. For a certain site having a distance x and $(l-x)$ to the nearest lines we have

$$Q_x=Q'(x)Q'(l-x) \tag{22}$$

for 2D growth where

$$\begin{aligned} Q'(x)&=\prod_{i=0}^{x+il\leqslant\lambda t} R(t,x+il) \\ &=\exp\left[-I\lambda t^2\sum_{i=0}^{x+il\leqslant\lambda t} f\left(\frac{x+il}{\lambda t}\right)\right] \end{aligned} \tag{23}$$

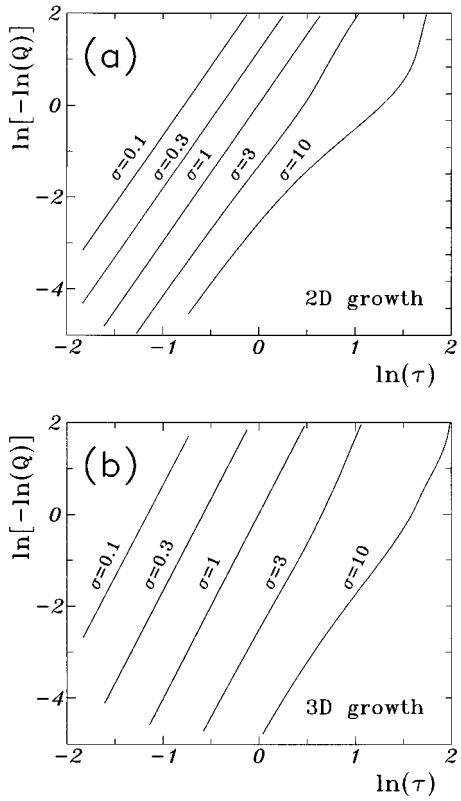

FIG. 4. Dependence of the mean survival probability Q on the reduced time $\tau=(I\lambda)^{1/2}t$ for varying $\sigma=(I/\lambda)^{1/2}l$, in the case of nucleation at line defect: (a) 2D growth; (b) 3D growth.

is considered. The mean survival probability is obtained by $Q=2/l\int_0^{l/2}Q_x dx$.

For 3D growth we may write

$$Q_{x,y}=Q''(x,y)Q''(l-x,y)Q''(l-x,l-y)Q''(x,l-y) \tag{24}$$

for a site in the position (x,y) to a nucleation line. Analogously we have here

$$Q''(x,y)=\prod_{i=0,j=0}^{(x+il)^2+(y+jl)^2\leqslant\lambda^2t^2} R[t,((x+il)^2+(y+jl)^2)^{1/2}]. \tag{25}$$

This yields the mean survival probability for the 3D lattice $Q=4/l^2\int_0^{l/2}\int_0^{l/2}Q_{x,y}dxdy$.

In Fig. 4 the dependence of the survival probability on the reduced time $\tau=(I\lambda)^{1/2}t$, the reduced distance between nucleation lines $\sigma=(I/\lambda)^{1/2}l$, and the degree of dimension (2D or 3D) is shown. Especially for $\sigma\leqslant 1$, strict linear behavior is present in the plot of $\ln[-\ln(t)]$ vs $\ln(\tau)$ with a slope of 3 for 2D and 4 for 3D growth.

B. Nucleation at planar grain boundary

Now we consider the case of preferred nucleation at a plane such as grain boundary in reality. For unit surface in the plane the nucleation rate is I as usual. As demonstrated in Fig. 5, an arbitrary site A has a distance $OA=y$ to the plane and thus $(x^2+y^2)^{1/2}$ to the site B in the plane for $OB=x$. If the site A remains untransformed at time t, the site B must be

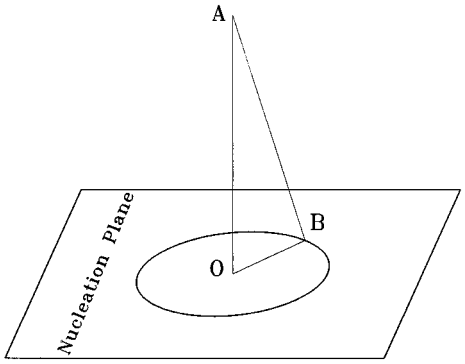

FIG. 5. Growth of grains nucleated at a planar grain boundary with constant rate.

untransformed up to $\tau=t-(x^2+y^2)^{1/2}/\lambda$. The total probability that the site A is untransformed at the time t is thus obtained,

$$R(t,y)=q_{k_0}\prod_{i=1}^{m} q_{k_i}^{2\pi i}. \tag{26}$$

Here k_i and m are the same as in Eq. (18b). This yields

$$R(t,y)=\exp\left\{-2\pi\int_0^{(\lambda^2t^2-y^2)^{1/2}}[\lambda t-(x^2+y^2)^{1/2}]\frac{I}{\lambda}xdx\right\}$$

$$=\exp\left[-\frac{\pi}{3}I\lambda^2t^3g\left(\frac{y}{\lambda t}\right)\right] \tag{27}$$

with $g(u)=1-3u^2+2u^3$. For the presence of more than one nucleation plane, we assume that totally K planes are homogeneously situated in the lattice. Following the same procedure as the foregoing section, we get the probability for a site to remain untransformed,

$$Q=\exp\left(\frac{2K}{L}\int_0^{\lambda t}\ln R(y)dy\right)$$

$$=\exp\left[-\frac{2\pi KD}{3L}I\lambda^3t^4\int_0^1 g(u)du\right]$$

$$=\exp\left[-\frac{\pi K}{3L}I\lambda^3t^4\right]. \tag{28}$$

By substituting $I'=KI/L$ we obtain

$$Q=\exp(-\pi I'\lambda^3t^4/3)$$

which is identical to Eq. (10). The kinetics is not altered by the randomly distributed boundaries as the nucleation source. If we assume that all nucleation planes are parallel arranged with distance l, for each site having distances x and $(l-x)$ both to the nearest planes we thus have $Q_x=Q'(x)Q'(l-x)$ with

$$Q'(x)=\exp\left[-\frac{\pi}{3}I\lambda^2t^3\sum_{i=0}^{x+il\leqslant\lambda t}g\left(\frac{x+il}{\lambda t}\right)\right]. \tag{29}$$

We are able to determine the mean survival probability for 2D nucleation and 3D growth by

$$\bar{Q}=\frac{2}{l}\int_0^{l/2}Q_x dx.$$

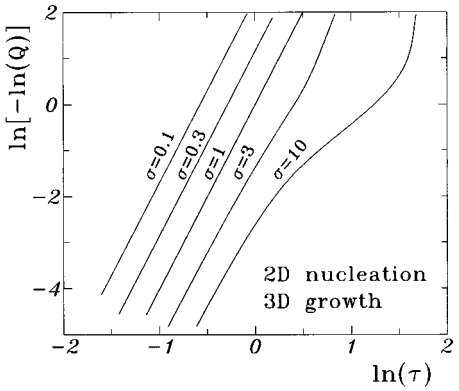

FIG. 6. Dependence of the mean survival probability Q on the reduced time $\tau=(\pi I\lambda^2/3)^{1/3}t$ for varying $\sigma=(\pi I/3\lambda)^{1/3}l$, in the case of 2D nucleation and 3D growth.

In Fig. 6 this mean survival probability is illustrated against the reduced time $\tau=(\pi I\lambda^2/3)^{1/3}t$. All curves in Fig. 6 have an initial slope of 4.

C. Nucleation in restricted zone

We consider at first the effect of a piece of the nucleation zone on the survival probability at the site O, as seen from Fig. 7(a). This nucleation zone is defined from x_1 to x_2 in x direction, but infinitely large in the y and z directions for the corresponding 2D or 3D problem. The probability of the site O not being transformed by the growth of grains nucleated in this piece of source considered is obtained by the following procedure:

$$Q'(t,x_1,x_2)=\exp\left(-\int_{V\{x_1,x_2\}}\int_0^{t-r/\lambda} I\,du\,dV\right). \tag{30}$$

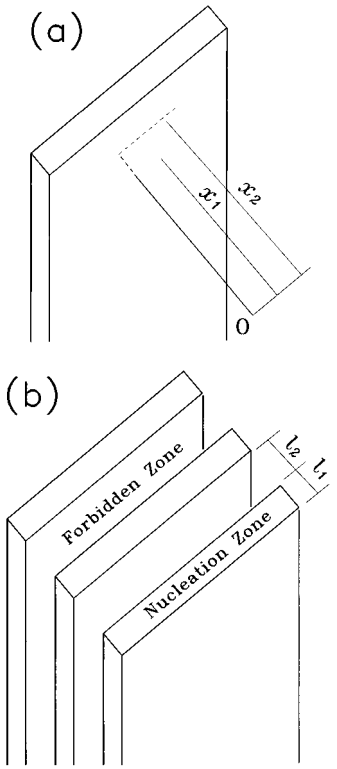

FIG. 7. Illustration of nucleation in restricted volume: (a) A a piece of nucleation zone; (b) periodically arranged nucleation zones.

The integration yields the solution

$$Q'(t,x_1,x_2)=\exp\left\{-I\lambda^D t^{D+1}\left[\chi\left(\frac{x_2}{\lambda t}\right)-\chi\left(\frac{x_1}{\lambda t}\right)\right]\right\}, \tag{31}$$

where $D=1,2,3$ are the degrees of dimension. Here we have

$$\chi(u)=\begin{cases}-\dfrac{1}{2}(1-u)^2, & \text{1D}\\[2mm] \dfrac{1}{3}\arcsin u+\dfrac{2}{3}u(1-u^2)^{1/2}-\dfrac{1}{3}u\,\ln(1+(1-u^2)^{1/2}/u), & \text{2D}\\[2mm] \dfrac{\pi}{6}(2u-2u^3+u^4), & \text{3D}\end{cases}. \tag{32}$$

The cases in which the whole lattice is composed of two zones periodically can be studied now. In one zone of length l_1 nucleation can take place with the rate I and in the other zone with size l_2 nucleation is forbidden, as shown in Fig. 7(b). In both zones the nuclei are allowed to grow with a constant rate λ.

For a site in the nucleation zone having a distance x from the boundary of both zones, we have

$$Q_1(x)=\exp\{-I\lambda^D t^{D+1}[W_1(t,x)+W_1(t,l_1-x)]\}. \tag{33}$$

$W_1(t,\eta)$ varies for three different cases. For $\lambda t<\eta$ we have

$$W_1(t,\eta)=\chi(1)-\chi(0). \tag{34a}$$

For $\lambda t>\eta$ we may set $\lambda t-\eta=n(l_1+l_2)+\delta$ with $0<\delta<l_1+l_2$. For $\delta<l_2$ it yields

$$W_1(t,\eta)=\chi\left(\frac{\eta}{\lambda t}\right)-\chi(0)+\sum_{i=0}^{n-1}\left\{\chi\left[\frac{\eta+(i+1)(l_1+l_2)}{\lambda t}\right]-\chi\left[\frac{\eta+l_2+i(l_1+l_2)}{\lambda t}\right]\right\}. \tag{34b}$$

For $\delta\geqslant l_2$ additional terms are inserted

$$W_1(t,\eta)=\chi(1)-\chi(0)+\chi\left(\frac{\eta}{\lambda t}\right)-\chi\left[\frac{\eta+n(l_1+l_2)}{\lambda t}\right]+\sum_{i=0}^{n-1}\left\{\chi\left[\frac{\eta+(i+1)(l_1+l_2)}{\lambda t}\right]-\chi\left[\frac{\eta+l_2+i(l_1+l_2)}{\lambda t}\right]\right\}. \tag{34c}$$

For a site in the forbidden zone having a distance y from the boundary, we have

$$Q_2(t,y)=\exp\{-I\lambda^D t^{D+1}[W_2(t,y)+W_2(t,l_2-y)]\}. \tag{35}$$

Also here three ranges are to be distinguished. We have for $\lambda t<\eta$,

$$W_2(t,\eta)=0, \tag{36a}$$

for $\lambda t-\eta=n(l_1+l_2)+\delta$ with $0<\delta<l_1$,

$$W_2(t,\eta)=\chi(1)-\chi\left[\frac{\eta+n(l_1+l_2)}{\lambda t}\right]+\sum_{i=0}^{n-1}\left\{\chi\left[\frac{\eta+l_1+i(l_1+l_2)}{\lambda t}\right]-\chi\left[\frac{\eta+i(l_1+l_2)}{\lambda t}\right]\right\}. \tag{36b}$$

and finally for $l_1\leqslant\delta<l_1+l_2$,

$$W_2(t,\eta)=\sum_{0}^{n}\left\{\chi\left[\frac{\eta+l_1+i(l_1+l_2)}{\lambda t}\right]-\chi\left[\frac{\eta+i(l_1+l_2)}{\lambda t}\right]\right\}. \tag{36c}$$

Integration over two zone yields the equation describing the mean survival probability

$$\bar{Q}=\frac{1}{l_1+l_2}\left(\int_0^{l_1}Q_1(x)dx+\int_0^{l_2}Q_2(y)dy\right). \tag{37}$$

Figure 8 shows curves for $\bar{Q}$ calculated by using Eq. (37) for many variations. The 1D, 2D, and 3D cases with different density of nucleation source are considered, whereas the ratio l_1/l_2 is fixed. It is observed, that in the plot of $\ln[-\ln(t)]$ vs $\ln(\tau)$ the slope of curves in the initial stage equals 2, 3, 4 for 1D, 2D, and 3D cases, respectively.

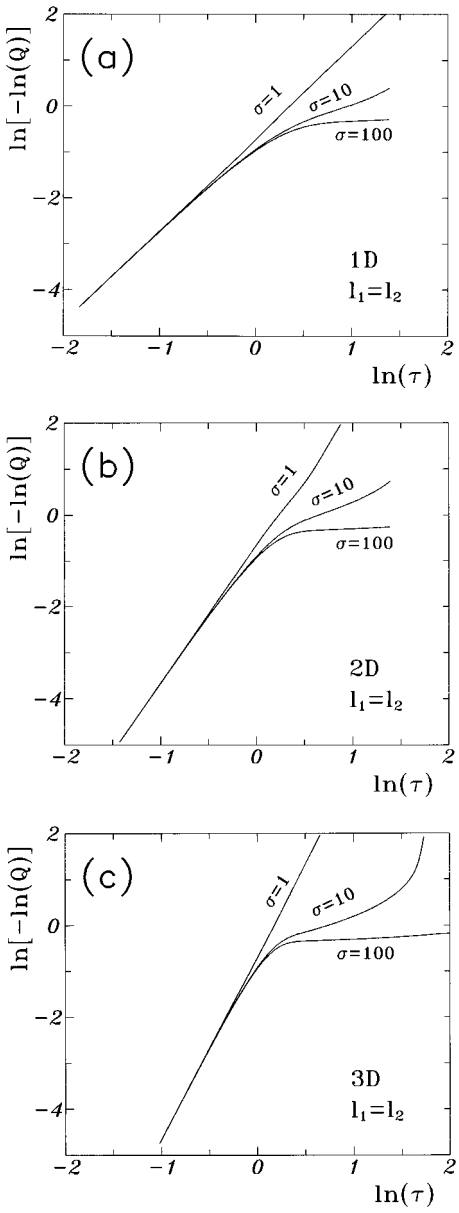

FIG. 8. Dependence of the mean survival probability Q on the reduced time τ for varying σ, in the case of periodically arranged nucleation zones: (a) 1D: $\tau=(I\lambda)^{1/2}t$, $\sigma=(I/\lambda)^{1/2}l$; (b) 2D: $\tau=(\pi I\lambda^2/3)^{1/3}t$, $\sigma=(\pi I/3\lambda)^{1/3}l$; (c) 3D: $\tau=(\pi I\lambda^3/3)^{1/4}t$, $\sigma=(\pi I/3\lambda)^{1/4}l$.

IV. DISCUSSION

Equations (6) and (10) describing the kinetics of the isothermal transformation in homogeneous 2D and 3D systems are obtained by following the probability calculation step by step. Compared to the classical derivation by Avrami,[2] in this treatment all quantities used are strictly defined and no concepts like phantom nuclei or extended regions are required, which makes the present derivation very transparent and easily understandable. Moreover, since analytical and numerical calculations of the survival probability are also applicable for finite and discrete systems and even for nonsteady conditions, the present method can be easily extended to the problems with nucleation rate and growth rate varying both with time and with space by considering the detailed atomistic properties.[2,3] For example, one of the interesting problems of the anisotropic growth, which leads to the development of texture during grain growth, will be discussed in our subsequent article.

Due to the direct algorithm of the present derivation, it is possible now to study the interference of many parallel processes. These relationships are revealed by Eqs. (15) and (17), which indicate that the superposition of more than one process may not lead to the change of the order of the reaction. A possible way to detect such interference in practice is to study the dependence of the mean grain size on the growth rate, which obeys the simple power law for the single process and the more complicated relation as Eq. (16).

Another very important feature of the probability calculation is that the correlation between two occurrences separated by time or by space can be investigated. From the two nuclei correlation the distribution of the nuclei pair with the separating distance is obtained as in Eq. (14). The curve in Fig. 2 clearly demonstrated that for the higher dimension the distribution becomes sharper, which is the natural consequence of the decay in the form of $\exp(-\tau^{D+1})$.

For the various problems of preferred nucleation studied in Sec. III, it is recognized that for l being the distance between the nucleation region it is the quantity $\sigma=A'(I/\lambda)^{1/(D+1)}l$ which determines the form of the transformation kinetics. In the case of strongly regular arrangement of nucleation region it is numerically illustrated in Figs. 4, 6, and 8 that for $\sigma\leqslant 1$, the order of the reaction $n=\partial \ln[-\ln(Q)]/\partial \ln t$ remains $D+1$. This is also analytically shown as Eq. (21) for the randomly varying σ. Especially for preferred nucleation at 1D or 2D defects, the phenomenological rate $\nu=-\partial \ln Q/\partial(t^n)$ is found to be proportional to the reciprocal of the mean distance of the nucleation region. This implies that for $\sigma\leqslant 1$ with sufficient high defect density, or high growth rate and low nucleation rate, we may use Eqs. (6) and (10) without respect to the detailed mechanism of the nucleation. For $\sigma>1$, all curves in Figs. 4, 6, and 8 appear to have a definite initial n with an initial linear period in the plotting of $\ln[-\ln(Q)]$ vs $\ln \tau$ for $\tau=A'(I\lambda^D)^{1/D+1}t$. In prolonged annealing the curves bend to the lower transformation rate. This slowing down of the transformation has been frequently observed in the previous experiments[4–6] and has not been convincingly explained in many cases.

V. CONCLUSION

The fundamentals of the present derivation have been introduced in the preceding article[1] for the simple 1D systems. Following the calculation of the survival probability step by step, the transformation with nucleation and growth mechanism in a homogeneous system during isothermal annealing is analytically solved for the general 2D and 3D cases. For the constant isotropic growth rate, the well-known Avrami equation is reestablished.

By the present direct method, the transforming probability in each small volume at any time interval can be definitely determined, so that it is possible to investigate the interfering processes. It is demonstrated that the superposition of these processes does not lead to a change in the order of reaction but in the dependence of the mean grain size on the growth rate. Also the correlation between different regions or many grains can be studied which allows the determination of the distribution of nuclei pairs with the separation distance.

Solutions for preferred nucleation in various special regions of 1D, 2D, and 3D are obtained. It is analytically or numerically demonstrated, that for randomly distributed nucleation regions or a relatively high density of these nucleation sources, the kinetics of the transformation is the same as the nucleation in the whole homogeneous volume. Furthermore, even for very low density of nucleation sources, an initial reaction order of $D+1$ is observed.

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