Kinetics of grain-boundary nucleated transformations in rectangular geometries and one paradox relating to Cahn’s model

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It was found by Jägle and Mittenmeijer [Acta Mater. 59 (2011) 5775-5786] as a result of computer simulations that Cahn’s equation underestimates pronouncedly the transformed fraction in reality. To test the hypothesis that a strong correlation in the arrangement of grains in the Cahn model (they are “tied” to planes) can be responsible for this phenomenon, the paradox of packing is described: the structures composed of the same elements (random parallelepipeds) transforming in the same way, but packed differently, give different transformation rates. One of these structures is a special Cahn model – the grain structure of parallelepipeds formed by three sets of random parallel planes orthogonal to each other. An alternative structure consists of the same parallelepipeds, but randomly packed; it looks like a real grain structure. It is shown analytically that the kinetics of transformation in the first structure is considerably slowed down in comparison with that in the second. For the various intermediate structures under consideration, the kinetic curves are between these two, so that the following rule is established: the transformation kinetics is accelerated, when the correlation in the arrangement of the parallelepipeds weakens. Preliminarily, volume-fraction expressions are obtained for the systems of an infinite number of parallel planes arranged both regularly and randomly. As a special case of random arrangement, a non-Poissonian point process (the second-order Erlang process) of arrangement of planes is considered for the first time. The exact volume-fraction expression obtained for this case shows that it cannot be derived by Cahn’s method, i.e. the extended-volume approach is applicable only to Poisson processes. The volume fraction equations for regular planes are used to study cubic grain structures, both regular and random. It is shown that Cahn’s equation underestimates the transformation kinetics in both regular and random structures with four different size distributions of cubes; the degree of underestimation depends on the size distribution, being the largest in the regular structure.
1. Introduction

The classical Kolmogorov-Johnson-Mehl-Avrami (KJMA) theory [1-5] solves the problem of calculating the volume fraction (VF) of a new phase in the process of crystallization under certain model assumptions. In view of the importance of this theory and its broad applications, the verification of underlying model assumptions and various extensions of the original theory, including extensions beyond its limitations, continued in recent decades [6-17]. While the VF is an integral quantity, a more detailed study of the transformation process and the resulting structure is performed using Secimoto’s [18] m-point correlation functions [19-23], microstructural descriptors [24-29], grain-size distribution functions [30-35], and other characteristics [36, 37]. Double-logarithmic VF plots, together with the corresponding temporal behavior of the Avrami exponent, provide information on the mechanisms of nucleation and growth.

One of the extensions of the KJMA theory is calculating the VF of a new phase nucleated at lower-dimension objects such as surfaces, lines, and points. Originally, this problem was first considered by Cahn [38] as applied to nucleation at faces, edges, and corners of grains in the framework of Avrami’s extended-volume concept [4, 5]; later, this model was revisited and generalized [7, 39-41]. It should be noted that VF calculation for progressive nucleation at points was done by Avrami himself [4, 5] who assumed that nucleation generally occurs by this mechanism. Some of the problems mentioned above, specifically, grain-size distribution and grain-boundary nucleated transformation were already considered by Johnson and Mehl [2]. In the latter case, they represented grains as equal spheres, and also assumed grains “isolated” from each other, when a growing nucleus cannot cross the grain boundaries. Later, Johnson and Mehl’s model was supplanted by Cahn’s one.

The model of spherical grains has recently been revisited and essentially improved [42]: firstly, the grains are not isolated from each other and are distributed in size; secondly, the rigorous critical-region (CR) method [6-8] which is a development of Kolmogorov’s one [1] was applied to obtain the VF expression for this system. The transformation kinetics (TK) is determined here (in addition to the distribution function) by the characteristic parameter $\bar{\alpha}$, which is the mean number of nuclei born on the boundary of the grain of mean size $\overline{R}_0$ for the time $t^* = \overline{R}_0 / u$, where $u$ is the nucleus growth velocity. It was shown that the TK in this model qualitatively differs from that of Cahn’s model. At large $\bar{\alpha}$ values, the double-logarithmic VF plot deviates from Cahn’s one and ends with a steep bend which corresponds to a sharp increase
in the Avrami exponent $n$ at the late stage, whereas $n \to 1$ in the Cahn model. This bend exists in two opposite cases - a very narrow ($\delta$-shaped) and a wide grain size distribution. It was shown by computer simulations [30, 35] and analytical calculations [2, 42] that a process with continuous nucleation results just in a wide grain size distribution. The similar form of double-logarithmic VF plots obtained by experimentalists for the crystallization of bulk metallic glasses [43] suggests that (i) these glasses have a grain structure (as opposed to the concept of homogeneous “frozen” liquid) and nucleation occurs at grain boundaries; (ii) this structure was formed as a result of continuous nucleation and growth of non-crystalline nuclei (clusters) [44, 45]. In this way, the results of the formal TK theory allow us to make important conclusions about the structure of matter and the way of its formation.

The different behavior of the Avrami exponents mentioned above is reflected in the behavior of the corresponding VFs. It was established for the first time by Jägle and Mittenmeijer [46] that the Cahn model underestimates pronouncedly the TK in reality. The present report aims to investigate in detail the cause of this phenomenon. The following two cases should be distinguished. (i) Comparison of the TK in any structure of identical elements of size $R_0$ (e.g., spheres) with the corresponding (i.e. containing the same $\omega$, the area of boundaries in unit volume) Cahn expression. (ii) Comparison of the TK in a structure of size-distributed elements with the corresponding Cahn expression. As grains are size-distributed in the Cahn model, the underestimation in the first case is easily explained by the contribution of large grains with $R > R_0$; just these grains delay the transformation process, “stretching” it in time. Cahn’s VF has the exponential tail $X_C(t) \to 1 - \exp(-2\omega t)$ originating from random planes and corresponding to $n = 1$, whereas the cubic-power asymptotics $X \to 1 - (1 - ut/R_0)^3$ holds in the system of identical elements at sufficiently large $\alpha$, values, giving a sharp increase in $n$ [42]. This case is also illustrated here by comparing the TK in regular and random structures of both plates and planes.

Cahn’s equation involves a single parameter $\omega$ which can be adjustable at a fixed $\bar{\alpha}$ value. However, the Avrami exponent does not depend on $\omega$; it is determined by the model itself and cannot be changed by a change in $\omega$ value. The latter only shifts the kinetic curve as a whole, so that it can intersect a comparing curve, underestimating it at the late stage due to the exponential tail [42]. So, the temporal behavior of the Avrami exponent in the model of spherical grains cannot be reproduced by any “corrected” Cahn equation in principle.

The second case is more complicated. First, it is unclear whether this underestimation is systematic (i.e. holds for all grain size distributions) or it is absent for some distributions. Second, as two size-distributed structures are compared, the reason for the underestimation is not
evident; individual grains in both structures are transformed in the same way. However, there is an essential distinction of the Cahn model from a real grain structure: the arrangement of grains in this model is strongly correlated - infinite arrays of grains are “tied” to their own planes. To understand how this correlation affects the TK and whether it is the cause of underestimation, it is necessary to compare Cahn’s TK with that in a grain structure with the same size distribution as in the Cahn model. However, this distribution is unknown and its obtaining is not an easy task.

Therefore, a particular Cahn model is considered here – the grain structure of random parallelepipeds which is formed by three sets of random planes orthogonal to each other. Since the TK in this model is described by the same equation as in the general Cahn model, both these models are physically equivalent, if they use the same $\omega$-value. However, all calculations, e.g., obtaining the grain size distribution, in the particular model are much simpler. The same parallelepipeds but repacked randomly form the grain structure similar to a real one; it has the same volume distribution of grains, as the initial structure. In this way, comparison of the TK in these two structures can be performed analytically, which is the subject of this paper.

The paper is organized as follows. In Section 2, the TK in the ensemble of both identical and width-distributed infinite plates is studied. The results of this Section are employed in Section 3, where the systems of an infinite number of parallel planes arranged either regularly or randomly are considered. The paradox of packing is described in details in Section 4. The TK in cubic structures, both regular and random, is studied in Section 5. Conclusions Section finalizes the paper.

2. Ensemble of width-distributed plates

Derivation of a VF equation in the process of surface-nucleated crystallization of an infinite plate of width $L = 2R_0$ can be performed by the CR method, similarly to the case of a spherical particle [42]. Details of such derivation can be found in Ref. [47]; the isothermal equation for the untransformed VF is obtained as follows:

$$Q^{(\omega)}(\tau) = \begin{cases} 
(1 - \tau) + \int_{1-\tau}^{1} e^{-\alpha_1 \phi_1(x,\tau)} \, dx, & \tau < 1 \\
\int_{0}^{\tau-1} e^{-\alpha_1 \phi_1(x,\tau)} \, dx + \int_{\tau-1}^{1} e^{-\alpha_1 \phi_1(x,\tau)} \, dx, & 1 \leq \tau \leq 2, \\
\int_{0}^{\tau} e^{-\alpha_1 \phi_1(x,\tau)} \, dx, & \tau > 2
\end{cases} \quad (1)$$

$$\phi_1(x,\tau) = \tau^3 - 3\tau(1 - x)^2 + 2(1 - x)^3$$
\[ \varphi_2(x, \tau) = 2\left[ \tau^3 - 3\tau(1 + x^2) + 6x^2 + 2 \right] \]

where \( \tau = ut / R_0 = 2ut / L \) and \( x = r / R_0 \) are the dimensionless time and distance, respectively;

\[ \alpha_s = (\pi / 3)(I_s / u)R_0^3 \]

is the characteristic parameter for given surface nucleation rate \( I_s \) and the nucleus growth velocity \( u \). The transformed VF is \( X^{(pt)}(\tau) = 1 - Q^{(pt)}(\tau) \). Differently from the case of a spherical particle, where the similar equations give the ensemble-averaged VF value, here this is an exact VF value of a plate; as the plate is infinite, \( Q(t) \) is a self-averaging quantity here [42], similarly to the case of KJMA model.

The same notations are used here as in Ref. [42] for ease of comparison and to demonstrate the generality of the approach employed. Isothermal equations for \( X^{(pt)}(t) \) were also obtained in Ref. [17] by the time-cone [48, 49] method; the results of numerical simulation of film transformation are reported in Ref. [50].

The equation for the untransformed fraction \( Q_s(\tau) \) of the surface itself is as follows:

\[
Q_s(\tau) = \begin{cases} 
  e^{-\alpha_s \tau^2}, & 0 < \tau \leq 2 \\
  e^{-2\alpha_s(\tau^3 - 6\tau + 8)}, & \tau > 2 
\end{cases}
\]  

(2)

It is seen that for \( \tau < 2 \) the law of plate-surface transformation is the same as the law of transformation of a single plane, as it must, whereas the case of \( \tau > 2 \) reflects the influence of another plane: at time \( \tau > 2 \) \( (ut > L) \), a nucleus appeared on one plane can cross another plane. So, the parameter \( \alpha_s \) characterizes the rate of surface transformation; the characteristic time of surface transformation is \( \tau_s \sim \alpha_s^{-1/3} \). The stage when the surface transformation is completed was called by Cahn the “saturation of boundaries” [38].

Defining by \( t' = R_0 / u \) the time corresponding to \( \tau = 1 \), the following representation for \( \alpha_s \) is obtained:

\[ \alpha_s = \frac{\pi}{3} I_s t' R_0^2 \]  

(3)

Hence, this parameter is proportional to the mean number of nuclei formed on the area \( R_0^2 \) during time \( t' \).

Later, the boundary saturation (BS) limit \( \alpha_s \rightarrow \infty \) will be essentially employed. In this limit, transformation proceeds by the 1D growth of the film formed on a plane at \( t' = 0 \). The BS-limit VF is

\[
X^{(pt)}_{BS}(\tau) = 1 - Q^{(pt)}_{BS}(\tau) = \begin{cases} 
  \tau, & \tau \leq 1 \\
  1, & \tau > 1 
\end{cases}
\]  

(4)
The BS-limit line \( X_{BS}^{(pt)}(r) \) is asymptotic for the kinetic curves \( X^{(pt)}(r) \) approaching it at large \( \alpha_s \) [47].

Introducing the corresponding bulk nucleation rate \( I_b = \omega_b I_s \), where \( \omega_b = 2/L = 1/R_0 \) is the mean area of plate surface in unit volume, we get the corresponding bulk-nucleation KJMA equation

\[
Q_k(r) = \exp \left( -\frac{1}{2} \alpha_s r^4 \right) \quad (5)
\]

The double-logarithmic VF plots together with the corresponding KJMA straight lines are shown in Fig. 1a; the plots are similar to those for spherical particles, in particular, they end with a steep bend at large \( \alpha_s \) values [42]. The corresponding temporal behavior of the Avrami exponent [47] also has common features.

Obviously, Eq. (1) can be also interpreted as the untransformed VF of the ensemble of identical parallel plates representing a regular 1D structure; the plates in this structure are isolated from each other, so that nuclei of one plate cannot intergrow into adjacent plates (this assumption is similar to that of Johnson-Mehl’s model for grain-boundary nucleated transformations [2, 3]).

To get the VF of the ensemble of width-distributed plates, we need the \( R_0 \)-dependent VF of a plate at a fixed time \( t \) [42]. It is obtained from Eq. (1) by substitutions

\[
\rho = \frac{1}{r} = \frac{R_0}{ut} = \frac{L}{2ut}, \quad y = \frac{r}{ut}, \quad x = \frac{y}{\rho} \quad (6)
\]

The characteristic dimensionless parameter here is \( \beta = (\pi/3)t\rho \}; \quad \alpha_s = \beta \rho^3 \). The result is as follows:

\[
Q^{(pt)}(\beta_s, \rho) = \left\{ \begin{array}{ll}
\frac{\rho - 1}{\rho} + \frac{1}{\rho} \int_0^\rho e^{-\beta_s \psi_1(y, \rho)} dy, & \rho \geq 1 \\
\frac{1}{\rho} \left\{ \int_0^1 e^{-\beta_s \psi_1(y, \rho)} dy + \int_1^\rho e^{-\beta_s \psi_1(y, \rho)} dy \right\}, & \frac{1}{2} < \rho < 1 \\
\frac{1}{\rho_0} \int_0^\rho e^{-\beta_s \psi_2(y, \rho)} dy, & 0 < \rho \leq \frac{1}{2}
\end{array} \right.
\]

\[
\psi_1(y, \rho) = 1 - 3(\rho - y)^2 + 2(\rho - y)^3 \\
\psi_2(y, \rho) = 2\left[ 1 - 3(\rho^2 + y^2) + 6\rho y^2 + 2\rho^3 \right]
\]

The dependence \( X^{(pt)}(\beta_s, \rho) = 1 - Q^{(pt)}(\beta_s, \rho) \) is monotonically decreasing and has the plateau \( X(\beta_s, \rho) = 1 \) at sufficiently large \( \beta_s \)s [47]. The BS-limit curve here is \( X_{BS}^{(pt)}(\rho) = 1/\rho \)
for $\rho \geq 1$ and $X_{BS}^{(\rho)}(\rho) = 1$ for $\rho < 1$ (cf. Eq. (4)); the VF curves approach it with increasing $\beta_s$

Let $f_2(L)$ be the probability density function for the plate width. The Erlang distribution

$$f_k^{(L)}(L) = \frac{\lambda^k (\lambda L)^{k-1}}{(k-1)!} e^{-\lambda L}$$  \hspace{1cm} (8a)$$

of the $k$-th order and its particular case of $k = 1$ - the exponential distribution

$$f_1^{(L)}(L) = \lambda e^{-\lambda L}$$  \hspace{1cm} (8b)$$
inherent in the Poisson process considered later - are employed hereafter. As is known, the sum

of $k$ random quantities distributed by the exponential law, Eq. (8b), is distributed by the $k$-th

order Erlang law, Eq. (8a).

The mean for $f_k^{(L)}(L)$ is $\bar{L}_k = k \lambda^{-1}$, so that $\bar{L}_1 = \lambda^{-1}$ for $f_1^{(L)}(L)$. Utilizing $\bar{L}_1$ as a

characteristic length, we shall use further the dimensionless width $l = L / \bar{L}_1 = L \lambda$ and the

dimensionless distributions

$$f_k(l) = \frac{l^{k-1}}{(k-1)!} e^{-l}$$  \hspace{1cm} (9a)$$

$$f_1(l) = e^{-l}$$  \hspace{1cm} (9b)$$

The probability for the point $O'$ to fall at random into a plate of the width $[L, L + dL]$
equals to the relative measure of these plates, according to the geometrical definition of

probability:

$$p_k(l)dl = \frac{L f_k^{(L)}(L)dl}{\bar{L}_k} = \frac{L f_k^{(L)}(L)dl}{\bar{L}_1} = \frac{l^k e^{-l} dl}{k!}$$  \hspace{1cm} (10a)$$

$$p_1(l)dl = l e^{-l} dl$$  \hspace{1cm} (10b)$$

These basic probabilities will be reused below.

Multiplying the above VF $Q^{(en)}(\beta_s, \rho)$ by $p_1(l)dl$ and integrating over the whole range

of $l$, we get the desired untransformed VF of the ensemble. Preliminarily, $\beta_s$ and $\rho$ are

represented as follows [42]:

$$b \equiv \frac{\pi \bar{T}_S}{3 \, u}, \quad \alpha_s = b R_0^3, \quad R_0 = \bar{L}_1 / 2, \quad \tau = \frac{ut}{R_0} = 2ut \bar{L}_1, \quad \beta_s = \alpha_s \tau^3, \quad \rho = \frac{R_0}{ut} = \frac{L}{2ut} = \frac{l}{\bar{T}}$$  \hspace{1cm} (11)$$

Finally,

$$Q_k^{(en)}(\bar{T}) = \int_0^\infty Q^{(en)}(\alpha_s \tau^3, \frac{l}{\tau}) p_k(l)dl, \quad X_k^{(en)}(\bar{T}) = 1 - Q_k^{(en)}(\bar{T})$$  \hspace{1cm} (12)$$

The BS-limit VF is
\[ Q_{\text{us}}^{(\alpha)}(\rho) = \frac{\rho - 1}{\rho} = 1 - \frac{\bar{\tau}}{\bar{\tau}} = Q_{\text{us}}^{(\alpha)}(l, \bar{\tau}), \quad l > \bar{\tau} \]  

(13a)

which is the untransformed part \( 1 - 2ut / L \) of the plate of width \( L \); \( Q_{\text{us}}^{(\alpha)}(l, \bar{\tau}) = 0 \) for \( l < \bar{\tau} \). The probability for the point \( O' \) to fall into the untransformed part of any plate, i.e. into the untransformed part of the ensemble is

\[ Q_k^{(\alpha)}(\bar{\tau}) = \int_{\tau}^{\infty} Q_{\text{us}}^{(\alpha)}(l, \tau) p_k(l) dl \]  

(13b)

In the two main variants considered here, \( k = 1 \) and \( k = 2 \), this gives

\[ Q_1^{(\alpha)}(\bar{\tau}) = \int_{\tau}^{\infty} \left( 1 - \frac{\bar{\tau}}{l} \right) e^{-\tau} dl = e^{-\tau} \]  

(14a)

\[ Q_2^{(\alpha)}(\bar{\tau}) = \frac{1}{2} \int_{\tau}^{\infty} \left( 1 - \frac{\bar{\tau}}{l} \right)^2 e^{-\tau} dl = \left( 1 + \frac{\bar{\tau}}{2} \right) e^{-\tau} \]  

(14b)

Fig. 1b shows how the width distribution slows down the TK as compared to the TK in the corresponding regular structure; the ensemble of identical plates with \( L = L_1 \) and hence \( \alpha_s = \alpha_s \), \( \tau = \bar{\tau} \) is employed for comparison. It is seen that the late-stage TK of the ensemble of exponentially distributed plates at \( \alpha_s = 10^3 \) is even slower than the TK of the ensemble of identical plates at \( \alpha_s = 0.1 \); the exponential tail of the former corresponds to \( n = 1 \), whereas \( n \to 3 \) for the latter [47]. Kinetics slows down to a greater extent with the increasing order \( k \) of Erlang’s distribution. Each kind of curves in Fig. 1b approach its BS-limit line corresponding to Eqs. (4), (14a) and (14b), at large \( \alpha_s, \alpha_s \) values. Obviously, the kinetics slows down due to the contribution of plates with \( L > L_1 \).

3. Infinite number of parallel planes

3.1. Regular arrangement

Here the periodic 1D structure of parallel planes with the same spacing \( L \) between them is considered, Fig. 2. Eq. (1) for one pair of planes consists of three time intervals. The sequential addition of new pairs of planes is accompanied by an increase in the number of time intervals in the VF equation, as well as the complication of the latter. Therefore, we should employ some approximation to get a VF equation for the system of an infinite number of planes. Here the same approximation is used, as in Ref. [42] for the model of grain-boundary nucleated transformations – it can be called the mean-field approximation (MFA). Marking out the pair
containing the random point $O'$ (Fig. 2), the influence of other (external) planes on transformation of the space bounded by this pair is represented as some effective bulk nucleation from the outside. Specifically, the computational procedure is as follows.

We specify the CR at time $t'$ for the point $O'$ taken at random at time $t$ - the sphere of radius $R(t', t)$ - and denote by $V_i(r; t', t)$ and $V_j(r; t', t)$ the volumes of spherical segments cut off by the right and left planes, respectively (Fig. 2);

\[
V_i(r; t', t) = \frac{\pi}{3} \left[ 2R^3(t', t) - 3(R_0 - r)R^2(t', t) + (R_0 - r)^3 \right],
\]

\[
V_j(r; t', t) = \frac{\pi}{3} \left[ 2R^3(t', t) - 3(R_0 + r)R^2(t', t) + (R_0 + r)^3 \right]
\]  

(15)

The mean area $S_i^{(e)}(r; t', t)$ of external planes within the segment of volume $V_i(r; t', t)$ is

\[
S_i^{(e)}(r; t', t) = \omega V_i(r; t', t)
\]  

(16a)

where $\omega$ is the mean area of planes in unit volume. We have for nucleation on external planes

\[
I_s S_i^{(e)}(r; t', t) = I_b \omega V_i(r; t', t) = I_b V_i(r; t', t), \quad I_b = \omega I_s
\]  

(16b)

where $I_b$ is the mean bulk nucleation rate. This equation means that nucleation on external planes can be represented as bulk nucleation outside the given pair of planes.

Further, the probability $Q^{(pl)}(r, t)$ for the point $O'$ to be untransformed at time $t$ is calculated following the procedure of deriving Eq. (1) which is complemented by the influence of external planes; the general nonisothermal equations are given in Ref. [47]. The isothermal VF equation is obtained as follows:

(1) $\tau < 1$:

\[
Q^{(pl)}(\tau) = (1 - \tau) + \int_{1-\tau}^{1} e^{-\phi_1(x, \tau) + \phi_i^{(e)}(x, \tau)} \, dx
\]  

(17a)

(2) $1 \leq \tau \leq 2$:

\[
Q^{(pl)}(\tau) = \int_{0}^{\tau-1} e^{-\phi_2(x, \tau) + \phi_i^{(e)}(x, \tau)} \, dx + \int_{\tau-1}^{1} e^{-\phi_1(x, \tau) + \phi_i^{(e)}(x, \tau)} \, dx
\]  

(17b)

(3) $\tau > 2$:

\[
Q^{(pl)}(\tau) = \int_{0}^{1} e^{-\phi_1(x, \tau) + \phi_i^{(e)}(x, \tau)} \, dx
\]  

(17c)

\[
\phi_1^{(e)}(x, \tau) = \frac{1}{2} \tau^4 - (1 - x)\tau^3 + (1 - x)^3 \tau - \frac{1}{2}(1 - x)^4
\]

\[
\phi_2^{(e)}(x, \tau) = \tau^4 - 2\tau^3 + 2(1 + 3x^2)\tau - (1 + 6x^2 + x^4)
\]
where the functions \( \varphi_i(x, \tau) \) are the same as in Eq. (1), whereas the functions \( \varphi^{(ex)}_i(x, \tau) \) represent the contribution of external planes. This contribution gives the characteristic parameter

\[
\alpha_b = \frac{\pi L_b R_u^4}{3 u} = c \alpha s, \quad c \equiv \omega R_0
\]

For \( n \) pairs of planes, \( \omega = 2n/(2n-1)L \), which gives \( \omega = 1/L \) in the limit \( n \to \infty \). Hence,

\[
c = R_0/L = 1/2.
\]

This is the 1D regular model of grain-boundary nucleated transformations. Fig. 3a displays the kinetic curves \( X^{(bi)}(\tau) \) in comparison with the VFs \( X^{(bi)}(\tau) \) for the ensemble of identical isolated plates, Eq. (1), for different \( \alpha_s \) s. As it was expected, \( X^{(bi)}(\tau) > X^{(bi)}(\tau) \) due to the effect of external planes; this effect is noticeable at small \( \alpha_s \) s and diminishes with their increase due to the developing BS phenomenon. The latter counteracts the influence of external planes, so that both dependences converge; it is seen that they are close already at \( \alpha_s = 1 \).

### 3.2. Random arrangement: the mean field approximation

Let the spacing \( L \) between planes be a random quantity with the probability density \( f^{(L)}(L) \). This case differs from the above case of the ensemble of width-distributed plates in that the “plates” are not isolated now, i.e. a nucleus born on any plane contributes to the transformation of the whole system (a growing nucleus can cross planes). This is the 1D random model of grain-boundary nucleated transformations. For calculating the VF here, the above time-dependent VF, Eqs. (17a-c), must be transformed to a \( R_0 \)-dependent VF, similarly to Eq. (7).

Substituting equalities (6) into Eqs. (17a-c), we get the characteristic parameter

\[
\beta_b = (\pi / 3)L_b u^4 \tau^4, \quad \alpha_b = \beta_b \rho^4
\]

and

\[
\beta_b = \beta_s \omega \tau = \beta_s \omega \sqrt{\beta_s / b}, \quad b \equiv \frac{\pi L}{3 u}
\]

Expressions of the form \( \beta_s [\psi_i(y, \rho) + \omega \sqrt{\beta_s / b} \psi^{(ex)}_i(y, \rho)] \) are obtained as arguments of exponential functions. Eq. (18a) can be further transformed using the characteristic length \( \bar{L}_1 \) and Eq. (11):

\[
\omega \sqrt{\beta_s / b} = \omega \bar{R}_0 \tau = \bar{\tau}, \quad \bar{\tau} = \omega \bar{R}_0
\]

As a result,

(1) \( \rho \geq 1 \):
\[ Q^{(pl)}(\beta, \rho, \tau) = \frac{\rho - 1}{\rho} + \frac{1}{\rho} \int_0^\rho e^{-\beta \psi_1^{(\gamma)}(y, \rho)} dy \]  

(19a)

(2) \( \frac{1}{2} < \rho < 1 \):
\[ Q^{(pl)}(\beta, \rho, \tau) = \frac{1}{\rho} \left[ \int_0^\rho e^{-\beta \psi_1^{(\gamma)}(y, \rho)} dy + \int_1^\rho e^{-\beta \psi_1^{(\gamma)}(y, \rho)} dy \right] \]  

(19b)

(3) \( 0 < \rho \leq \frac{1}{2} \):
\[ Q^{(pl)}(\beta, \rho, \tau) = \frac{1}{\rho} \int_0^\rho e^{-\beta \psi_1^{(\gamma)}(y, \rho)} dy \]  

(19c)

\[ \psi_1^{(\gamma)}(y, \rho) = \frac{1}{2} (\rho - y) (\rho - y)^3 - \frac{1}{2} (\rho - y)^4 \]

\[ \psi_2^{(\gamma)}(y, \rho) = 1 + 2 \rho (\rho^2 + 3y^2 - 1) - (\rho^4 + 6y^2 \rho^2 + y^4) \]

Similarly to Eq. (12), the desired VF equation for the considered system in the MFA is
\[ Q_\xi^{(\alpha)}(\tau) = \int_0^\infty Q^{(pl)}(\bar{\alpha}, \bar{\tau}^3 \frac{1}{\tau}, \bar{\tau}) p_k(l) dl \]  

(20)

It will be shown later that
\[ \omega = \hat{\lambda} = \bar{L}_i^{-1} \]  

(21)

for the exponential distribution \( f_i(l) \); hence, \( \bar{c} = \omega \bar{R}_0 = \bar{R}_0 / \bar{L}_i = 1/2 \) in this case. However, \( \bar{c} \) can be different for another application of Eqs. (19a-c) considered later.

It should be noted that the influence of external planes discussed above is absent in the BS limit, so that the same results take place for the ensemble of width-distributed plates and for the ensemble of random planes; in particular, Eqs. (14a, b) hold for random planes as well.

Fig. 3b shows kinetic curves for regular and the corresponding random planes with the exponential distribution (the 1D Cahn model); the correspondence is provided by the equality \( \lambda^{-1} = L_i = L \), from where \( \bar{\tau} = \tau \) and \( \bar{\alpha}_i = \alpha_i \). Cahn’s curves largely underestimate those for regular planes; the divergence between them increases with an increase in \( \alpha_i \). At \( \alpha_i = 10^4 \), each curve practically coincides with its BS-limit one, Eq. (4) for \( X^{(pl)}_{1,BS}(\tau) \) and \( X^{(mf)}_{1,BS}(\tau) = 1 - \exp(-\tau) \).

These equations explain the mentioned divergence: all Cahn’s curves end with the exponential tail, which is not the case of regular-planes curves.

### 3.3. Random arrangement: exact solution
The system of random parallel planes with the Poisson distribution in space allows an exact solution for the VF which can be obtained by the CR method of Ref. [7]. This fact is valuable to estimate the MFA accuracy.

Preliminarily, we find the probability \( q_p(r, t) \) for the point \( O' \) to be untransformed at time \( t \) from the plane at a distance \( r \) from it. Evidently, the condition \( r < R_m(t) = R(0, t) \) must be satisfied; otherwise, \( q_p(r, t) = 1 \). As follows from earlier studies [7, 47], the result is

\[
q_p(r, t) = \exp \left[ - \int_0^t I_s(t') S(r; t', t) \, dt' \right], \quad S(r; t', t) = \pi [R^2(t', t) - r^2]
\]  

(22a)

where \( t_m(r, t) \) is determined by the equality \( R(t_m, t) = r \). In the isothermal case, this gives

\[
q_p(x, t) = e^{-\beta_s |x| - 3x^2/2} \quad x = r / R_m(t) = r / ut \quad \beta_s(t) = (\pi/3) I_s u^2 t^3
\]  

(22b)

As before, we take at random a point \( O' \) in the considered system, Fig. 4, and find the probability \( Q(t) \) that it is untransformed at time \( t \). The CR for the point \( O' \) at time \( t' = 0 \) is the sphere of radius \( R_m(t) \). Let it be intersected by \( n \) planes. The diametrical line intersects these planes at points \( C_1, C_2, \ldots, C_n \) representing the Poisson point process (P-process). Denoting by \( r_k = |O'C_k| \) the distance from the point \( O' \) to the \( k \)th plane, \( k = 1, 2, \ldots, n \), the probability \( q_n(r_k, t) \) for the point \( O' \) to be untransformed at time \( t \) at the given \( n \) and realization of the set \( \{r_k\} = \{r_1, r_2, \ldots, r_n\} \) is found as a product of the probabilities \( q_p(r_k, t) \), Eq. (22a):

\[
q_n(\{r_k\}, t) = \prod_{k=1}^n q_p(r_k, t) = \prod_{k=1}^n \exp \left[ - \int_0^t I_s(t') S(r_k; t', t) \, dt' \right]
\]  

(23a)

This equation reflects the possibility for a growing nucleus to cross planes, which is the property of Cahn’s model [38]. Due to this property, the transformations of the point \( O' \) from different planes are independent events, which results in the product (23a).

The desired function \( Q(t) \) is obtained by averaging \( q_n(\{r_k\}, t) \) over all \( r_k \)-values and \( n \):

\[
Q(t) = \sum_{n=0}^\infty P_\text{i}(n) \int_0^{R_m(t)} \cdots \int_0^{R_m(t)} q_n(\{r_k\}, t) \phi(r_1, r_2, \ldots, r_n) \, dr_1 dr_2 \ldots dr_n, \quad P_\text{i}(n) = \frac{(\bar{n})^n}{n!} e^{-\pi}
\]  

(23b)

where \( \phi(\{r_k\}) \) is the distribution density of the set \( \{r_k\} \) and \( P_\text{i}(n) \) is the Poisson distribution.

The positions \( r_k \) of the points \( C_k \) are independent random quantities uniformly distributed on the segment \([AB] \), Fig. 4, at the condition that their number on this segment is \( n \) [51], which is an important property of the P-process. According to the independency,
\( \phi(r_1, r_2, \ldots, r_n) = \tilde{\phi}(r_1)\tilde{\phi}(r_2)\ldots\tilde{\phi}(r_n) \). According to the uniformity, the probability for the point \( C_k \) to be in the interval \( dr_k \) equals to \( dr_k / 2R_m \), where \( 2R_m \) is the length of the segment \([AB]\). With respect to the point \( O' \), the point \( C_k \) can be at the right or at the left at the same distance \( r_k \) (two equal possibilities), hence, this probability is doubled and \( \tilde{\phi}(r_k)dr_k = dr_k / R_m \), \( \tilde{\phi}(r_k) = 1 / R_m \). As a result, the \( n \)-fold integral in Eq. (23b) equals to \( w(t)^n \), where

\[
w(t) = \frac{1}{R_m(t)} \int_0^{R_m(t)} q_p(t, r)dr = \int_0^1 q_p(x, t)dx
\]  

(24)

Averaging with the Poisson distribution yields

\[
Q_{(1)}(t) = \sum_{n=0}^{\infty} \frac{n^n}{n!} e^{-\bar{n}} w(t)^n = e^{-\bar{n}(1-w(t))}
\]

(25)

The mean number \( \bar{n} \) of points on the segment \([AB]\) of length \( 2R_m(t) \) in the P-process with the intensity \( \lambda \) is

\[
\bar{n} = 2\lambda R_m(t)
\]  

(26)

The mean area of the plane part located inside the CR is

\[
\bar{S} = \pi \int_0^{R_m(t)} (R_m^2 - r^2) \frac{dr}{R_m} = \frac{2}{3} \pi R_m^2
\]  

(27a)

Hence, the mean area of planes in unit volume is

\[
\omega = \frac{\bar{S}}{(4\pi / 3)R_m^3} = \frac{\bar{n}}{2R_m}
\]  

(27b)

from where

\[
\bar{n} = 2\omega R_m(t)
\]  

(28)

Comparing to Eq. (26), we get the equality \( \omega = \lambda \) used above, Eq. (21).

Finally, isothermal Eq. (25) has the following explicit form:

\[
Q_{(1)}(t) = \exp\left\{ -2\omega t \int_0^1 \left[ 1 - e^{-\beta_s(t)(1-3x^2+2x^4)} \right] dx \right\}
\]  

(29a)

which is the Cahn equation [38, 41]. The result is clear, as the basic probability \( q_p(t, r) \) depends only on the distance \( r \) to a plane, but not on its orientation. The given case can be considered as the 1D Cahn model.

Denoting, as before, \( \tau = 2\omega t = 2ut\lambda \) and \( \beta_s = \alpha_s \tau^3 \), we get

\[
Q_{(1)}(\tau) = \exp\left\{ -\tau \int_0^1 \left[ 1 - e^{-\beta_s(t)(1-3x^2+2x^4)} \right] dx \right\}, \quad X_{(1)}(\tau) = 1 - Q_{(1)}(\tau)
\]  

(29b)
From the above equations, the extended volume \( X_e^{(1)}(\tau) \) of Cahn’s theory [38] can be represented as

\[
X_e^{(1)}(\tau) = \bar{\tau}(1 - w(\bar{\tau})) \quad w(\bar{\tau}) = \int_0^1 e^{-Ax^2} dx
\] (30)

In the BS limit, \( \bar{\tau} \to \infty \), one obtains \( w(\bar{\tau}) \to 0 \) and

\[
X_{e,BS}^{(1)}(\tau) = \bar{\tau}, \quad Q_{1(i)}^{(BS)}(\tau) = e^{-\tau}, \quad X_{1(i)}^{(BS)}(\tau) = 1 - e^{-\tau}
\] (31)

in accordance with Eq. (14a). The exponential in these equations takes into account the overlap of growing plates; the quantity \( \bar{\tau} \) can be also interpreted as the volume of growing and overlapping plates in unit volume of the system, by definition. This overlap can be neglected at \( \bar{\tau} \to 0 \); then \( X_{1(i)}^{(BS)}(\bar{\tau}) = X_e^{(1)}(\bar{\tau}) = \bar{\tau} \).

It should be also noted that \( \bar{n} = \bar{\tau} \), according to Eq. (26), so that \( P_{(i)}(n) = P_{(i)}(n, \tau) \).

3.4. Random arrangement: non-Poissonian distribution

A non-Poissonian distribution of planes is of great interest; apparently it was not considered in literature as yet in connection with TK. Intervals between the successive events (points) in the P-process are independent and have the same exponential distribution \( f_1^{(L)}(L) \), Eq. (8b). An evident and important generalization is obtained under the assumption that these intervals are independent and have the same distribution \( f^{(L)}(L) \) different from the exponential one. The resulting series of point events on the time axis is called the renewal process; these processes are studied in the renewal theory [52, 53] which is a section of the theory of reliability of technical devices. One of the instances is the \( k \)-th-order Erlang point process (E\( k \)-process), \( k > 1 \); it is obtained from the P-process as result of its thinning out, when each \( k \)-th event of the P-process is retained and all other events are removed.

As a simplest example of a non-Poissonian distribution of planes, the E\( 2 \)-process is considered here; it is obtained as a result of thinning out the P-process, when each second plane is removed. The intervals between the remaining planes (similar to the inter-arrival times in the renewal theory) are distributed according to the second-order Erlang law \( f_2^{(L)}(L) \), Eq. (8a) with \( k = 2 \). As follows from the previous Section, all we need to derive the VF \( Q_{(2)}(t) \) in this case is an expression for \( P_{(2)}(n) \), the probability of \( n \) points on the given segment \( [AB] \), and the distribution \( \Phi(t) \) of these points.

The probability \( P_{(i)}(x) \) of \( n \) points on the segment \([0,x]\) is calculated in Ref. [47]:
\[ P_n(x) = e^{-\lambda x} \left\{ \frac{1}{2} \frac{(\lambda x)^{2n+1}}{(2n+1)!} + \frac{(\lambda x)^{2n}}{(2n)!} + \frac{1}{2} \frac{(\lambda x)^{2n-1}}{(2n-1)!} \right\}, \quad n = 1, 2, 3, \ldots \]  

(32a)

\[ P_n(x) = e^{-\lambda x } \left( 1 + \frac{1}{2} \lambda x \right) \]  

(32b)

It is seen that the probability \( P_n(x) \) is the sum of three Poisson probabilities: one for even \((2n)\) number of points and two for odd numbers \((2n-1)\) and \((2n+1)\); the latter enter with the weighting factor \(1/2\). Such expression structure reflects the fact that \( n \) points on the segment \([0,x)\) in the given \(E_2\)-process can be obtained as result of thinning out the parent \(P\)-process containing on the segment \([0,x)\) either \(2n-1\), \(2n\), or \(2n+1\) points.

The segment \([0,x)\) used in calculations is the segment \([AB]\) here, i.e. \( x = 2R_m(t) = 2ut \), \( \lambda x = 2ut\lambda = \bar{r} \). The mean \( \bar{\pi}(x) \) in the considered process, as is shown \(ibid\), equals to \( \lambda x/2 = \lambda R_m(t) \); comparing this equation to Eq. (28) which is valid in the given case as well, we get

\[ \omega = \frac{\lambda}{2} \]  

(33)

for the \(E_2\)-process, which is an expected result, since the number of planes is twice less than in the parent \(P\)-process.

In view of the above relations, Eqs. (32a, b) acquire the following form

\[ P_{(2)}(n) = P_{(2)}(n, \bar{r}) = e^{-\bar{r}} \left\{ \frac{1}{2} \frac{\bar{r}^{2n+1}}{(2n+1)!} + \frac{\bar{r}^{2n}}{2(2n)!} + \frac{1}{2} \frac{\bar{r}^{2n-1}}{2(2n-1)!} \right\}, \quad n = 1, 2, 3, \ldots \]  

(34a)

\[ P_{(2)}(0, \bar{r}) = e^{-\bar{r}} \left( 1 + \frac{1}{2} \bar{r} \right) \]  

(34b)

Obviously, the \( n \) points remaining after the thinning procedure retain both the mentioned properties of the parent \(P\)-process – independence and uniformity; hence, the \( n \)-fold integral in Eq. (23b) equals to \( w(t)^{n} \), as before, where \( w(t) \) and \( w(\bar{r}) \) are given by Eqs. (24) and (30). In this way,

\[ Q_{(2)}(\bar{r}) = \sum_{n=0}^{\infty} P_{(2)}(n, \bar{r}) w^{n} = P_{(2)}(0, \bar{r}) + e^{-\bar{r}} \left\{ \frac{1}{2} \sum_{n=1}^{\infty} \frac{(\sqrt{w(\bar{r})})^{2n+1}}{(2n+1)!} + \frac{\sqrt{w(\bar{r})}^{2n}}{2(2n)!} + \frac{1}{2} \sum_{n=1}^{\infty} \frac{(\sqrt{w(\bar{r})})^{2n-1}}{2(2n-1)!} \right\} \]  

(35a)

These are series for hyperbolic sine and cosine, so that finally

\[ Q_{(2)}(\bar{r}) = e^{-\bar{r}} \left\{ \frac{1}{2} \left[ \sqrt{w(\bar{r})} + \frac{1}{\sqrt{w(\bar{r})}} \right] \sinh(\sqrt{w(\bar{r})} \bar{r}) + \cosh(\sqrt{w(\bar{r})} \bar{r}) \right\} \]  

(35b)
In the BS limit, we have \( W \to 0 \), \( \sinh(\sqrt{W} \tau) / \sqrt{W} \to \tau \), and \( \cosh(\sqrt{W} \tau) \to 1 \), so that the preexponential factor becomes equal to \( (1 + \tau / 2) \) and Eq. (35b) goes to Eq. (14b), as it must.

It is seen that Eqs. (14a) and (14b) coincide with the probabilities \( P_{(1)}(0, \tau) \) and \( P_{(2)}(0, \tau) \) of the absence of points on the segment \([AB]\) in the P- and E\(_2\)-process, respectively. Equivalently, these are probabilities that no plane intersects the CR. Indeed, the plane located at the distance \( R_m(t) = ut \) from the point \( O' \) (at either the point \( A \) or \( B \)) transforms it just at time \( t \) in the BS limit, whereas a plane located at \( r_k < ut \) transforms the point \( O' \) before time \( t \).

Hence, the CR has not to be intersected by planes to keep the point \( O' \) untransformed at time \( t \) in the BS limit. This result can be directly applied to the site-saturated nucleation on a straight line with the density \( \Lambda \) of nucleation sites. With the notation \( \tilde{\tau} = 2\Lambda ut \), the KJMA equation is \( X_K(\tilde{\tau}) = 1 - \exp(-\tilde{\tau}) \) in this case. If the nucleation sites represent the E\(_2\) process, then the VF equation is \( X_E(\tilde{\tau}) = 1 - (1 + \tilde{\tau} / 2)\exp(-\tilde{\tau}) \).

Denoting by \( \chi(\tau) \) the preexponential expression in Eq. (35b), we have

\[
X_{(2)}(\tau) = 1 - Q_{(2)}(\tau) = 1 - \exp[-X_{e(2)}'(\tau)], \quad X_{e(2)}'(\tau) \equiv \tau - \ln \chi(\tau) \tag{36a}
\]

\[
\frac{dX_{(2)}(\tau)}{d\tau} = (1 - X_{(2)}(\tau)) \frac{dX_{e(2)}'(\tau)}{d\tau} \tag{36b}
\]

These are familiar equations of the JMA extended-volume approach [2-5, 38]; \( X_{e(2)}'(\tau) \) is the “extended volume” for the E\(_2\)-process. In the BS limit, \( X_{e,BS}^{(2)}(\tau) = \tau - \ln(1 + \tau / 2) \), from where

\( X_{e,BS}^{(2)}(\tau) = X_{K}^{(BS)}(\tau) = \tau / 2 \) at \( \tau \to 0 \), which is twice less than \( X_{(1)}^{(BS)}(\tau) = X_{e,BS}^{(1)}(\tau) = \tau \) in the P-process due to the twice less number of planes here.

The extended volume \( X_e^{(1)}(\tau) \) expression, Eq. (30), was derived by Cahn [38] from clear geometrical constructions and it has a proper interpretation; as is mentioned above, \( X_e^{(1)}(\tau) = \tau \) is the volume of overlapping plates in unit volume of the system, in accordance with the extended volume definition. Similarly, the extended volume in the JMA theory is the volume of overlapping spherical nuclei. It is seen that the “extended volume” \( X_{e,BS}^{(2)}(\tau) \) of the E\(_2\)-process involves a logarithmic summand and therefore does not have the same interpretation as \( X_{e,BS}^{(1)}(\tau) \); it is only clear that \( X_{e,BS}^{(2)}(\tau) < X_{e,BS}^{(1)}(\tau) \) due to the more rare arrangement of planes. The \( X_{e(2)}'(\tau) \) expression is much more complex than \( X_e^{(1)}(\tau) \) one and has no clear geometrical interpretation, differently from the latter; therefore, it cannot be derived by the method of work [38]. So, Cahn’s method is successful only in the P-process and not applicable to non-Poissonian
ones. On the contrary, the present method as more rigorous and general allows us to get exact solutions for these processes as well.

Fig. 5a shows the kinetic curves \( X_{(i)}(\tau) \) and \( X_{(2)}(\tau) \) at small and large \( \alpha_s \) s. The TK is slower for the E\(_2\)-process, as it must. At large \( \alpha_s \) s, each kind of curves approach its BS-limit line \( X_{(k)}^{BS}(\tau) \), Eqs. (14a, b).

Figs. 5b and 5c give a comparison of the exact, \( X_{(k)}(\tau) \), and MFA, \( X_{(k)}^{MF}(\tau) \), curves for the P- and E\(_2\)-process, respectively. As it can be seen, the MFA is surprisingly good for the P-process and somewhat worse for the E\(_2\)-one; MFA equations slightly overestimate the exact kinetics, which is a clear result. The accuracy improves with increasing \( \alpha_s \) values obviously due to the developing BS phenomenon counteracting the influence of external planes; when the effect of external planes diminishes, the MFA and exact solutions give close results. The error given by the MFA in each process, \( \Delta X_{(k)}(\tau) = X_{(k)}^{MF}(\tau) - X_{(k)}(\tau) \), in the region of small \( \alpha_s \) s is shown in Fig. 5d. The error behavior is not monotonic with \( \alpha_s \) change; \( \Delta X_{(k)}(\tau) \) has a maximum at \( \alpha_s \sim 10^{-3} \). The maximal error in VF cubes \( \Delta X_{(i)}^{MF}(\tau) = (Q_{(i)}(\tau))^3 - (Q_{(i)}^{MF}(\tau))^3 \) is about 0.01; this fact will be used later.

4. Structures of random parallelepipeds: paradox of packing

4.1. Basic structure

Three sets of random parallel planes orthogonal to each other form the grain structure consisting of random parallelepipeds (hereafter, pp-s for brevity), Fig. 6a; let \( L_x, L_y, \) and \( L_z \) denote the pp edges. The randomness of pp-s should be clarified in more detail. If we take at random one pp, its edges \( (L_x, L_y, L_z) \) are independent random quantities. However, all the pp-s forming one plate between the neighboring planes, say, \( XY \), have the same \( L_z \)-value. Similarly, the pp-s forming rectangular cylinders have the same values of pairs, say, \( (L_x, L_y) \). In other words, there is a strong correlation in the arrangement of pp-s here; this fact is crucial for further consideration.

To get the VF of untransformed material in this structure, we take at random the point \( O' \) and calculate the probability \( Q_{(o)}(t) \) that it is untransformed at time \( t \). Evidently, \( Q_{(o)}(t) \) is found as the product of three probabilities to be untransformed in each set of parallel planes, in view of the independence of these events. If the planes in each of three sets are distributed
according to the P-process with the same parameter $\lambda$, then $Q_{(a)}^{(l)}(t) = Q_{(i)}^{(l)}(t)^3$, where $Q_{(i)}^{(l)}(t)$ is given by Eq. (29a), and

$$Q_{(a)}^{(l)}(\tau) = Q_{(i)}^{(l)}(\tau)^3 = \exp\left[-3\tau\int_0^1 \left[1 - e^{-\tau r^3(1-3x^2+2x^4)}\right]dx\right], \quad X_{(a)}^{(l)}(\tau) = 1 - Q_{(a)}^{(l)}(\tau) \quad (37)$$

i.e. the area $\omega_{pp}$ of boundaries in unit volume here is three times greater: $\omega_{pp} = 3\omega$. Similarly, $Q_{(a)}^{(2)}(\tau) = Q_{(2)}^{(l)}(\tau)^3$ for the E2-process.

The volume distribution of pp-s is of interest; it will be essentially used later. Having a pp ($L_x, L_y, L_z$), the task is to find the distribution of the product $L_x L_y L_z = V$ for known distributions $f^{(l)}(L_i)$ of the quantities $L_i, i = x, y, z$. At first, we find the distribution function $G(V)$ as the probability for the point ($L_x, L_y, L_z$) to be under the surface $L_x L_y L_z = V$, by definition:

$$G(V) = P\{L_x, L_y, L_z < V\} = \int_0^V dL_x \int_0^{V/L_x} dL_y \int_0^{L_y} f^{(l)}(L_x)f^{(l)}(L_y)f^{(l)}(L_z) \quad (38a)$$

Further, the desired probability density function $g^{(V)}(V)$ is obtained by differentiating:

$$g^{(V)}(V) = \frac{dG(V)}{dV} = \int_0^V dL_x \int_0^{V/L_x} dL_y \frac{1}{L_x L_y} f^{(l)}(L_x)f^{(l)}(L_y)f^{(l)}\left(\frac{V}{L_x L_y}\right) \quad (38b)$$

We can take the most general probability densities $f^{(l)}(L_i)$ as the $k_i$ th order Erlang laws with different $\lambda$, s:

$$f^{(l)}(L_i) = f_k^{(l)}(L_i) = \frac{\lambda^k_i L_i^{k_i-1}}{(k_i-1)!} e^{-\lambda_i L_i}, \quad i = x, y, z \quad (39)$$

The above $Q_{(a)}(t)$ can be easily obtained for all combinations with $k_i = 1, 2$ and different $\lambda$, s as a product of the corresponding 1D VFs. Combining different $k_i$ s with different $\lambda$, s in Eq. (39), we can model numerous pp structures with the exact probability density $g^{(V)}(V)$ for them. Any real grain distribution can be also fitted by the function $g^{(V)}(V)$ with properly chosen parameters $k_i$ and $\lambda_i$. Structures with strongly different $\lambda$, s or/and $k_i$ s will contain pp-s with strongly different $\bar{L}_i$, e.g., the plate-like pp-s ($L_x, L_y >> L_z$) or wire-like ones ($L_x, L_y << L_z$).

Here $\bar{\lambda}_i = \lambda$ and $k_i = k$ are used for simplicity; Eq. (38b) in this case is as follows:

$$g^{(V)}(V) = \frac{\lambda^3}{((k-1)!)^3} \int_0^V dL_x \int_0^{V/L_x} dL_y \frac{(\lambda V)^{k-1}}{L_x L_y} e^{-\lambda L_x + L_y + V/L_x L_y} \quad (40a)$$

Going to the dimensionless variables $l_i = L_i/\lambda$, $\nu = L^3 V$, $g(\nu) = \lambda^3 g^{(V)}(V)$, one obtains finally...
Defining the length \( l \) by relation \( \nu = l^3 \), the distribution over \( l \) is obtained as
\[
g_k^{(\nu)}(l) = 3l^2g_k(l^3) \tag{40c}
\]

### 4.2. Derivative structures

#### 4.2.1. Preliminary remarks

In what follows, an alternative way for deriving the VF equation is employed. The probability \( Q_{(a)}(t) \) that the random point \( O' \) at time \( t \) falls into the untransformed part of the system is obtained as the averaging product of two probabilities: (i) the probability \( dQ_{pp}(L_x, L_y, L_z) \) for the point \( O' \) to fall into a pp with the edges \([L_i, L_i + dl_i], i = x, y, z, \) and (ii) the probability \( q_{pp}(L_x, L_y, L_z; \tau) \) to fall into the untransformed part of this pp. Let the parallel planes forming the basic structure of Fig. 6a (hereafter called the (a)-structure) be distributed according to the P-process with the same parameter \( \lambda \); the considered further derivative structures retain this property (the index (1) at the VF is omitted).

In this way, one obtains for the (a)-structure in the dimensionless variables \( l_i = \lambda L_i \),
\[
\tau = 2ut \lambda
\]
\[
dQ_{pp}^{(a)}(l_x, l_y, l_z) = p_l(l_x)p_l(l_y)p_l(l_z)dl_xdl_ydl_z \tag{41a}
\]
\[
Q_{(a)}(\tau) = \int_0^\infty \int_0^\infty \int_0^\infty dl_x dl_y dl_z q_{pp}(l_x, l_y, l_z; \tau) l_x l_y l_z e^{-(l_x + l_y + l_z)} \tag{41b}
\]

This integral is the probability for the point \( O' \) to fall into the untransformed part of any pp, i.e. into the untransformed part of the whole system. In view of the independence condition,
\[
q_{pp}(l_x, l_y, l_z; \tau) = q_{pp}(l_x, \tau)q_{pp}(l_y, \tau)q_{pp}(l_z, \tau) \tag{42}
\]

for the (a)-structure, where \( q_{pp}(l_i, \tau) \) is the conditional probability for the point \( O' \) to be untransformed in the set of parallel planes at the condition that it is located between two planes separated by the distance \( l_i \). Here equations for \( q_{pp}(l_i, \tau) \) are the same, hence
\[
Q_{(a)}(\tau) = \left( \int_0^\infty q_{pp}(l, \tau) l e^{-l} dl \right)^3 \tag{43}
\]
For the structures considered below, either Eq. (42) does not hold or equations for $q_{pp}(l, \bar{r})$ are not the same and calculating some of them is a complicated procedure resulting in a cumbersome expression. Fortunately, such exact or MFA equations for $q_{pp}(l, \bar{r})$ are unnecessary for understanding the main idea of the present approach, so that the BS limit is further employed for $q_{pp}(l_x, l_y, l_z; \bar{r})$. In this limit,

$$q_{pp}(l_x, l_y, l_z; t) = \begin{cases} \frac{(L_x - 2ut)(L_y - 2ut)(L_z - 2ut)}{L_x L_y L_z}, & l_x, l_y, l_z \geq 2ut \\ 0, & \text{otherwise} \end{cases}$$

(44a)

In the dimensionless variables,

$$q_{pp}(l_x, l_y, l_z; \bar{r}) = \begin{cases} \left(1 - \frac{\bar{r}}{l_x}\right)\left(1 - \frac{\bar{r}}{l_y}\right)\left(1 - \frac{\bar{r}}{l_z}\right), & l_x, l_y, l_z \geq \bar{r} \\ 0, & \text{otherwise} \end{cases}$$

(44b)

So, both the separation given by Eq. (42) always holds and equations for $q_{pp}(l, \bar{r})$ are the same in the BS limit; they have a simplest form, $q_{pp}(l, \bar{r}) = 1 - \bar{r} / l$. Eq. (43) gives in this limit

$$Q_{(a)}(\bar{r}) = \left(\int_2^{\infty} \left(1 - \frac{\bar{r}}{l}\right)e^{-l} dl\right)^3 = e^{-3\bar{r}}$$

(45)

in accordance with Eq. (14a); this result is also obtained from Eq. (37) at $\alpha_s \to \infty$. In this Section, the superscript (BS) is omitted for brevity.

The derivative structures obtained from the (a)-one are as follows.

4.2.2. Structures with one and two degrees of freedom

(b)-Structure is obtained from the (a)-one by shifting the rectangular cylinders $(L_x, L_z)$ relatively each other along the $Y$-axis at random distances, Fig. 6b. As a result, only two sets of parallel planes, $XY$ and $YZ$, remain and there is no more the set of parallel planes $XZ$. Now the above probability $dQ_{pp}(L_x, L_y, L_z)$ for the point $O'$ to fall into the pp $(L_x, L_y, L_z)$ is calculated differently from case (a). The probabilities of $L_x$ and $L_z$ are calculated, as before:

$$p_1(L_x)p_1(L_z)dL_xdL_z$$ - this is the probability for the point $O'$ to fall into the rectangular cylinder $(L_x, L_z)$. The probability of the remaining quantity $L_y$ does not equal to $p_1(L_y)dL_y$, since there is no parallel planes $XZ$ here; this is simply the probability for the random quantity $L_y$ to be in the interval $[L_y, L_y + dL_y]$ which is determined as $f_y(l_y)dL_y$ by definition. The difference from
case (a) is as follows. Consider the subset of the same cylinders \((L_x, L_y)\). The point \(O'\) being in any of them has the same \(L_y\)-value in case (a) and different \(L_y\)-values in case (b); the probabilities of these values in each case are given above. This means that transition from (a)- to (b)-structure weakens the correlation in the arrangement of pp-s mentioned above by one step (with respect to \(L_y\) only) and therefore the (b)-structure is a structure with one “degree of freedom”. Finally,

\[
dQ^{(b)}_{pp}(l_x, l_y, l_z) = p_i(l_z) p_1(l_z) dl_z dl_y f_i(l_y) dl_y
\]

(46a)

and

\[
Q_{(b)}(\tau) = \left( \int \frac{1 - \frac{\tau}{l_z}}{l_z} e^{-\tau} dl_z \right) \left( \int \frac{1 - \frac{\tau}{l_y}}{l_y} e^{-\tau} dl_y \right) = e^{-\tau} \left[ e^{-\tau} + \tau \text{Ei}(\tau) \right], \quad \text{Ei}(\tau) = \int_{-\infty}^{\tau} \frac{e^x}{x} dx \quad (46b)
\]

where \(\text{Ei}(x)\) is the integral exponent.

Fig. 6c shows the formation of (c)-structure from the base (a)-one: the plates between the neighboring planes \(XY\) are shifted relatively each other along both the \(X\) and \(Y\) axes at random distances. As a result, only one set of parallel planes, \(XY\), remains. In this way, the probability of \(L_z\) is calculated here as \(p_i(L_z) dL_z\) and the probabilities of \(L_x\) and \(L_y\) as \(f_i(L_x) f_i(L_y) dL_x dL_y\).

Consider the subset of plates with the same width \(L_z\). The point \(O'\) being in any of them has the same \(L_x, L_y\)-values in case (a); indeed, to get the desired pp \((L_x, L_y, L_z)\), we take the cylinder \((L_x, L_y)\) and cut off its parts of width \(L_z\) by planes \(XY\). At the same time, the point \(O'\) has different pairs \((L_x, L_y)\) in case (c). In this way, transition from (a)- to (c)-structure weakens the correlation in the arrangement of pp-s by two steps (with respect to both \(L_x\) and \(L_y\)) and therefore the (c)-structure is a structure with two “degrees of freedom”. With respect to the (b)-structure, the correlation is weakened by one step more.

Finally,

\[
dQ^{(c)}_{pp}(l_x, l_y, l_z) = p_i(l_z) dl_z f_i(l_y) dl_y
\]

(47a)

\[
Q^{(c)}(\tau) = \left( \int \frac{1 - \frac{\tau}{l_z}}{l_z} e^{-\tau} dl_z \right) \left( \int \frac{1 - \frac{\tau}{l_y}}{l_y} e^{-\tau} dl_y \right) = e^{-\tau} \left[ e^{-\tau} + \tau \text{Ei}(\tau) \right] \quad (47b)
\]

4.2.3. Completely uncorrelated structure

As follows from the above consideration, the remaining step in the weakening of correlation is to destroy the set of parallel planes of the (c)-structure. In this way, we decompose
the base (a)-structure into single pp-s and then repack them randomly, Fig. 8d; this is the (d)-structure. As there are no parallel planes here, a length \( l \) (the spacing between planes) is no longer a basic measure for calculating the probability for the random point \( O' \) to fall into a certain region; the pp volume \( \nu \) is a basic measure here. The probability for the point \( O' \) to fall into a pp of volume \( \nu \) is the relative measure of these pp-s, by definition:

\[
P_i(\nu)d\nu = \frac{\nu g_i(\nu)d\nu}{\int_0^\infty \nu g_i(\nu)d\nu}
\]

(48)

where \( g_i(\nu) \) is given by Eq. (40b) with \( k = 1 \).

Having a given volume \( \nu \), the pp can have two arbitrary edges \( l_x \) and \( l_y \) with the probabilities \( f_i(l_x)dl_x \) and \( f_i(l_y)dl_y \); the third edge is \( l_z = \nu/l_xl_y \). As before, the untransformed part \( q_{pp}(l_x,l_y,l_z;\bar{\tau}) \) of the pp at time \( \bar{\tau} \) depends on these lengths:

\[
q_{pp}(l_x,l_y,l_z;\bar{\tau}) = \begin{cases} 
\frac{1}{\nu}(l_x-\bar{\tau})(l_y-\bar{\tau})\left(\frac{\nu}{l_xl_y} - \bar{\tau}\right), & l_x,l_y,\nu/l_xl_y \geq \bar{\tau}, \\
0, & \text{otherwise}
\end{cases}
\]

(49)

In this way,

\[
dQ^{(d)}_{pp}(l_x,l_y,\nu) = P_i(\nu)d\nu f_i(l_x)f_i(l_y)dl_xdl_y
\]

(50a)

\[
Q^{(d)}_{pp}(\bar{\tau}) = \int_\tau^\infty dl_x\int_\tau^\infty dl_y f_i(l_x)f_i(l_y)\int_{\pi_{l_xl_y}}^\infty q_{pp}(l_x,l_y,\nu;\bar{\tau})P_i(\nu)d\nu
\]

\[
= \int_\tau^\infty dl_x\int_\tau^\infty dl_y(l_x-\bar{\tau})(l_y-\bar{\tau})e^{-(l_x+l_y)}\left\{\frac{1}{l_xl_y}\int_{\pi_{l_xl_y}}^\infty P_i(\nu)d\nu - \bar{\tau}\int_{\pi_{l_xl_y}}^\infty \frac{P_i(\nu)d\nu}{\nu}\right\}
\]

(50b)

Evidently, the given approach with the probability \( P_i(\nu) \) cannot be applied to the (a)-structure for calculating \( dQ^{(a)}_{pp} \), where the probability for the point \( O' \) to fall into any pp of volume \( \nu \) is different – pp-s of the same volume \( \nu \) have different sets \((l_x,l_y,l_z)\) and the probability \( dQ^{(a)}_{pp}(l_x,l_y,l_z) \) is determined just by these sets, rather than by \( \nu \), Eq. (41a). The same holds for the (b)- and (c)-structures. The converse statement is also true: the approach of case (a) is not applicable to case (d), since there are no parallel planes here. Among the considered structures, evidently, the (d)-structure corresponds to a real grain structure. Just the difference in equations for the probabilities \( dQ^{(d)}_{pp} \) and \( dQ^{(a)}_{pp} \) underlies the difference in the real TK and that of Cahn’s model, as is discussed below. However, differently from the (a)- and (d)-structures having the same volume distribution of grains, in reality the grain size distributions in the structure under consideration and Cahn’s model are different. This fact modifies the mentioned
effect, giving different degrees of underestimation depending on the grain size distribution; this phenomenon is described in the next Section.

The kinetic curves \( X_{(\alpha)}(\tau) = 1 - Q_{(\alpha)}(\tau) \), \( \alpha = a, b, c, d \), are shown in Fig. 7a. It is seen that the sequential weakening of correlation from (a) to (d) accelerates the TK; it is the fastest in the completely uncorrelated (d)-structure and the slowest in the (a)-structure which is a particular case of Cahn’s model. Interestingly that curve (c) is very close to curve (d); the maximal difference between them is about \( 8 \times 10^{-3} \), which means that the correlation already in the (c)-structure can be thought weak.

In this way, the structures consisting of the same pp-s, but differently packed, give different rates of transformation; this phenomenon is called here the paradox of packing. It explains why the general Cahn model underestimates the real TK [46]. Although the planes in this model are at random angles, there is a strong correlation in the arrangement of polyhedra, similarly to the (a)-structure – each array of polyhedra is tied to a certain plane; each polyhedron belongs to several such arrays, as each pp in the (a)-structure belongs to three arrays of pp-s. As shown above, the Cahn equation with \( \omega_c = 3\lambda \) is the same as the (a)-structure VF equation, i.e. the particular and general Cahn models with the same \( \omega_c \) value give the same TK and therefore are indistinguishable from the physical point of view. The exponential asymptotics of Cahn’s equation corresponding to the 1D growth (\( n = 1 \)) originates just from random planes and therefore is closely related to the mentioned correlation. The real transformation curves (at a finite \( \alpha_s \)) approach those of Fig. 7a with increasing \( \alpha_s \), as in previous figures.

It is seen from the foregoing that a mathematical reason for the difference in kinetic curves (a)-(d) is different probabilistic measures \( dQ_{pp}^{(\alpha)} \), similarly to the classical Bertrand paradox [54]. From the physical point of view, different patterns of space filling occur in these cases. The space is filled by three sets of growing plates in case (a), by two sets of plates and single transforming pp-s in case (b), by one set of plates and single pp-s in case (c), and only by single transforming pp-s in case (d). To understand how single transforming pp-s accelerate the TK, the (C)- and (B)-structures corresponding to the (c)- and (b)-ones can be considered. The (C)-structure is simply the system of parallel planes with the exponential distribution of spacing between them, i.e. when the plates in the (c)-structure are not divided into pp-s; as shown above, the BS-limit kinetic curve here is \( X_{(C)}(\tau) = 1 - \exp(-\tau) \). If rectangular cylinders in the (b)-structure are not divided into pp-s, we get the (B)-structure; obviously, \( X_{(B)}(\tau) = 1 - \exp(-2\tau) \).

Comparing \( X_{(b)}(\tau) \) to \( X_{(B)}(\tau) \) and \( X_{(c)}(\tau) \) to \( X_{(C)}(\tau) \) in Fig. 7a, we see how the presence of
pp-s accelerates the TK; the difference between curves (C) and (c) is especially sharp. As curves (c) and (d) are close, this comparison sheds light on the result obtained for the (d)-structure.

4.2.4. Intermediate structures

In addition to the main (a)-(d)-structures described above, different intermediate structures can be considered as well. One of them, the (c')-structure, is shown in Fig. 6c'; the difference from the (c)-structure is in that the blocks of two adjacent plates are shifted relatively each other, rather than single plates. Of course, this classification is conditional: if extreme cases (a) and (d) are considered as main, then the (b)- and (c)-structures are also intermediate.

Let \( l = \lambda L \) is the block width, Fig. 6c'; it is distributed according to the second-order Erlang law. The probability for the point \( O' \) to fall into the pp \((l_x, l_y, l)\) is given by equation similar to Eq. (47a), but with \( p_2(l) dl \), Eq. (10a) with \( k = 2 \), instead of \( p_1(l_z) dl_z \):

\[
dQ_{pp}^{(c)}(l_x, l_y, l) = p_2(l) df_1(l_z) f_1(l_z) dl_x dl_y, \quad p_2(l) = \frac{l^2 e^{-l}}{2}
\]  (51a)

Hence, Eq. (47b) is replaced by the following one:

\[
Q_{(c')}(\tau) = c'(\tau) \left[ e^{-\tau} + \tau \text{Ei}(-\tau) \right] \]  (51b)

where \( c'(\tau) \) is the probability for the point \( O' \) to be in the untransformed part of the length \( l \); in the case when the length \( l \) is not separated into two parts, \( c'(\tau) \) is given by Eq. (14b). In the given case, calculations are more complicated.

The untransformed part of the length \( l \) is calculated differently for different \( l_z \)-values of one of the pp-s constituting the block; the possible three variants are shown in Fig. 8. The quantity \( l_z \) is limited now by the condition \( l_z \leq l \), so that its distribution \( f_1(l_z) \) must be normalized in accordance with this condition:

\[
\tilde{f}_1(l_z, l) = z(l) e^{-l_z}, \quad z(l) = \left( \int_0^l e^{-l_z} dl_z \right)^{-1} = \left( 1 - e^{-l} \right)^{-1}
\]  (52)

The mentioned three variants are as follows.

(i) \( 0 < L_z < 2ult \) \( (0 < l_z < \bar{\tau}) \)

The untransformed part here is

\[
\frac{L - L_z - 2ult}{L} = 1 - \frac{l_z + \bar{\tau}}{l}
\]  (53a)

In this way, the probability of variant (i) is
and the probability for the point to fall into the pp \((l, l', l')\) is given by:
\[
c'_i(\tau) = 2 \int_0^\tau d\tau' \int_{l_i+\tau}^{\infty} dl \left(1 - \frac{l_i + \tau}{l}ight)p_2(l)z(l)
\] (53b)

(ii) \(2ut < L_z < L - 2ut \quad (\overline{\tau} < l_z < l - \overline{\tau})\)

In this case, the untransformed region consists of two parts:
\[
\frac{(L - L_z - 2ut) + (L_z - 2ut)}{L} = 1 - \frac{2\overline{\tau}}{l}
\] (54a)

Changing the order of integration,
\[
\int_0^\infty \int_{l_i + \tau}^{\infty} dl \int_{l_z}^{\infty} dz = \int_0^\infty \int_{l_z}^{\infty} dz \int_{l_i + \tau}^{\infty} dl
\]

one obtains
\[
c'_i(\tau) = \int_{l_z}^{\infty} dz \int_{l_i + \tau}^{\infty} dl \left(1 - \frac{2\overline{\tau}}{l}ight)p_2(l)z(l)
\] (54b)

(iii) \(L - 2ut < L_z < L \quad (l - \overline{\tau} < l_z < l)\)

Going to the new variable \(l'_z = l_z - (l - \overline{\tau})\), \(0 < l'_z < \overline{\tau}\), we get the untransformed part as follows:
\[
\frac{L_z - 2ut}{L} = \frac{l_z - l + \overline{\tau}}{l} = 1 - \frac{2\overline{\tau} - l'_z}{l}
\] (55a)

The probability of this variant is
\[
c'_i(\tau) = \int_0^{l'_z} dl'_z \int_{l'_z + \tau}^{\infty} dl \left(1 - \frac{2\overline{\tau} - l'_z}{l}ight)e^{-(l - \overline{\tau})}p_2(l)z(l)
\] (55b)

Finally, the desired function \(c'(\tau)\) is the sum of these three,
\[
c'(\tau) = c'_i(\tau) + c'_i(\overline{\tau}) + c'_i(\tau)
\] (56)

It turns out that \(c'_i(\tau)\) is a monotonically decreasing function (from 1 to 0), whereas \(c'_i(\tau)\) and \(c'_i(\tau)\) are bell-shaped with maximum values 0.3 and 0.04, respectively. In this way, the first two summands give the main contribution to the sum; the smallness of \(c'_i(\tau)\) is evidently due to large \(l_z\) - values in this case and hence the exponentially small their probabilities.

Similarly, the (b')-structure can be formed, if the \(2 \times 2\) blocks of rectangular cylinders are shifted relatively each other in Fig. 6b, rather than single cylinders; let \(l^{(x)} = \lambda L^{(x)}\) and \(l^{(z)} = \lambda L^{(z)}\) be the block sizes distributed according to the second-order Erlang law. The probability for the point \(O'\) to fall into the pp \((l^{(x)}, l_z, l^{(z)})\) is
\[
dQ_{pp}^{(x)}(l^{(x)}, l_z, l^{(z)}) = p_2(l^{(x)})p_2(l^{(z)})dl^{(x)}dl^{(z)}f_1(l_y)dl_y
\] (57a)

and
Numerous intermediate structures can be constructed in the similar way by increasing the block sizes (as well as considering $k \times m$ blocks in case (b'), $k$ - and $m$ -blocks in case (c'), etc.), however, the complexity of analytical calculations also increases. All these structures differ from each other by the degree of correlation in the arrangement of pp-s. E.g., the degree of correlation in the structure of $k \times k$ blocks which generalizes the (b')-one increases with increasing $k$ and approaches that of the base (a)-structure. In this way, the degree of correlation in the (c')- and (b')-structures is slightly greater, than in the corresponding (c)- and (b)-structures, hence, the TK should be slightly slower. At first glance, it seems that the kinetic curves $X_{(c')}(\tau)$ and $X_{(c')}(\tau)$ coincide in Fig. 7a. However, there is still the small differences $\Delta X_{(c-c')} = X_{(c')}(\tau) - X_{(c')}(\tau)$ between them shown in Fig. 7b; the maximum of $\Delta X_{(c-c')}$ is about $10^{-3}$, whereas the maximum of the difference $\Delta X_{(b-b')} = X_{(b')}(\tau) - X_{(b')}(\tau)$ is four times greater. The smallness of $\Delta X_{(c-c')}$ was expected due to the small correlation in the (c)-structure itself. As is mentioned above, these differences will increase with increasing the block sizes.

5. Cubic structures

5.1. Regular cubic structure and its derivatives

A regular cubic structure is formed by three sets of regular parallel planes considered in Section 3.1. Obviously, the MFA untransformed VF in this structure is

$$Q^{(c)}(\tau) = (c'(\tau))^3[e^{-\tau} + \tau Ei(-\tau)]$$  \hspace{1cm} (57b)

as a consequence of the independency of events for the point $O'$ to be untransformed from each set; $Q^{(pl)}(\tau)$ is given by Eqs. (17a-c).

From this base (a)-structure, we can form the (b)-(d)-structures in the same manner, as in the previous Section. To understand the TK in these structures, the interpretation of Fig. 2 should be somewhat changed. Let this figure depicts the transformation of a single plate under the influence of some external surfaces. The parallel planes as such surfaces are employed in Fig. 2, however, the result, Eqs. (17a-c), depends only on the area $\omega$ of these surfaces in unit volume; hence, we can use *arbitrary surfaces* instead of planes in the MFA. Three mutually orthogonal plates, each with its environment, form a cube with some resulting environment; the VF of this cube in the MFA is given by Eq. (58). Let $\omega^{(c)}$ be the area of boundaries in unit volume for the
(a)-(d) structures; evidently, \( \omega^{(c)} = 3 \omega = 3/L = 3/2R_0 \) for the base (a)-structure. Being an average quantity, by definition,
\[
\omega^{(e)} = \lim_{V \to \infty} \frac{S(V)}{V} \tag{59}
\]
it has the same value for the (a)-(c) structures, despite the fact that cubes have different surrounding surfaces in these structures. Due to the independence of this environment stated above, the MFA TK in these structures is the same and given by Eq. (58). In particular,
\[
X^{(e)}_{\text{CS}}(\tau) = \begin{cases} 1 - (1 - \tau)^3, & \tau \leq 1 \\ 1, & \tau > 1 \end{cases} \tag{60}
\]
in the BS limit, when cubes are “isolated” from each other.

The (d)-structure consisting of randomly packed cubes may contain a void between them depending on the packing algorithm. The condition of minimum void can be imposed to get the random dense packing of cubes. The presence of a void affects the \( \omega^{(c)} \) value for this structure and therefore the TK; with the use of \( \omega^{(e)} \) as an input parameter, Eq. (58) with \( \omega = \omega^{(e)}/3 \) in the equation for \( Q^{(p)}(\tau) \) describes the TK in this structure as well. So, the results given below for a regular cubic structure take place for any system of identical cubes with the same \( \omega^{(c)} \) value.

Consider the spheres of radius \( R_0 = L/2 \) inscribed in the cubes of the base (a)-structure; they form the lattice of spheres dual to the given cubic lattice. It was shown [42] that
\[
c^{(e)} = \omega^{(e)} R_0 = \pi/2 = 1.57 \text{ for this spherical lattice, whereas } c^{(e)} = \omega^{(c)} R_0 = 1.5 \text{ for the given (a)-structure.} \tag{59}
\]
Fig. 9 displays kinetic curves for the regular cubic structure (or its derivative structures, in view of the above arguments), together with the curves for the dual structure of spheres and the corresponding Cahn equation which is Eq. (37) due to the equalities \( L = \lambda^{-1} \), \( \omega^{(e)} = 3/L = 3\lambda \); just this \( \omega^{(e)} \) value is substituted into Cahn’s equation giving
\[
2 \omega^{(e)} \alpha u t = 2(3\alpha)u t = 3\tau . \text{ The curves for cubes and spheres are close already at } \alpha_s \sim 0.1 ; \text{ the difference between them vanishes at large } \alpha_s ; \text{ This difference becomes noticeable only in the region of small } \alpha_s , \text{ where its behavior is not monotonic with a change in } \alpha_s , \text{ as in Fig. 5d; the maximal divergence is 0.08 at } \alpha_s \sim 10^{-3} . \text{ The limit } \alpha_s \to 0 \text{ corresponds, in particular, to } R_0 \to 0 \text{, which means that the system becomes homogeneous and both the types of curves should follow the KJMA kinetics in this limit [28, 29, 42]. It turns out that the condition of homogeneity is more inherent in spherical geometry; the kinetic curve for spheres practically coincide with the KJMA one } X_{K}(\tau) = 1 - \exp(-c^{(e)}\alpha_s \tau^4) \text{ already at } \alpha_s \sim 10^{-3} , \text{ whereas the corresponding curve for}
cubes still slightly overestimates these two. So, the difference in geometries manifests itself only in the region of small $\alpha_s$. As the kinetic curves for cubes were calculated in the MFA, it would be reasonable to use the MFA Cahn curves for comparison. However, as is seen from Fig. 5d (bottom solid lines), the difference between the MFA an exact Cahn curves is less than 0.01 even at small $\alpha_s$, so that exact Eq. (37) is employed. Cahn’s model noticeably underestimates the TK in the cubic structure. As is mentioned above, this occurs due to the quite different long-time asymptotics in both the models; the exponential asymptotics with $n \to 1$ takes place in Cahn’s model. In the cubic structure, $n \approx 4$ at small $\alpha_s$ (as in the case of spheres [42]) and $n$ increases sharply for Eq. (60) at large $\alpha_s$.

### 5.2. Random cubic structures

Developing further the present approach, we can obviously apply it to the (d)-structure with size-distributed cubes; Eqs. (19a-c) are used for this purpose. Having

$$Q_c(\beta_c, \rho, \bar{\tau}) = [Q^{(\rho)}(\beta_c, \rho, \bar{\tau})]^3$$

for a single cube of size $\rho$ in the system, one obtains for the whole system [42]

$$Q^{(c)}(\bar{\tau}) = \frac{\int_{0}^{\infty} Q_c(\alpha_c, \bar{\tau}, \bar{\tau}) f(l) dl}{\int_{0}^{\infty} f(l) dl}$$

where $f(l)$ is the size distribution of cubes.

The area of boundaries in unit volume is

$$\omega^{(c)} = \frac{6}{2} \frac{\int_{0}^{\infty} L^2 f(L) dL + \frac{1}{2} S_v}{\int_{0}^{\infty} L^3 f(L) dL + V_v}$$

(63a)

where $V_v$ and $S_v$ are the volume of voids and their total surface area, respectively; these voids are inevitable in a random structure. Cubes touch each other at faces; hence, the integral twice takes into account the area of grain boundaries and therefore is divided by two. As is seen from this equation, the volume and surface effects of voids on the $\omega^{(c)}$ value counteract to each other, so that the following estimate for $\omega^{(c)}$ is employed here for calculations:
$$\omega^{(c)} = 3 \frac{\int_{0}^{\infty} L^2 f(L) dL}{\int_{0}^{\infty} L^3 f(L) dL}$$ (63b)

Considering $\omega^{(c)}$ as an input parameter, the $\omega = \omega^{(c)}/3$ value is used in the equations for $Q_i^{(p)}(\beta, \rho, \tau)$. For the regular structure, $f(L) = \delta(L)$, Eq. (63b) gives $\omega^{(c)} = 3/L$.

The quantity $\omega^{(c)}$ is not needed in the BS limit, where Eq. (62) is as follows:

$$Q_{c,BS}(\tau) = \frac{\int_{0}^{\infty} (1 - \frac{\tau}{L})^3 f(l) dl}{\int_{0}^{\infty} f(l) dl}$$ (64)

The first distribution of interest is that corresponding to the random pp-s of Fig. 6a; the correspondence of a pp to the cube of the same volume is given by Eq. (40c). The distributions $g_{x}(\nu)$ and $g_{k}^{(i)}(l)$ are shown in Fig. 10 for some $k$ values; the function $g_{x}(\nu)$ is monotonically decreasing, whereas others have a maximum. In this way,

$$\omega_{k}^{(c)} = 3 \lambda \frac{\int_{0}^{\infty} l^2 g_{k}^{(i)}(l) dl}{\int_{0}^{\infty} l^3 g_{k}^{(i)}(l) dl} = 3 \lambda \gamma_{k}, \quad \bar{\omega}^{(c)} = \omega_{k}^{(c)}/R_0 = \frac{\omega_{k}^{(c)}}{2\lambda} = \frac{3}{2} \gamma_{k}$$ (65)

and $c = \bar{\omega}^{(c)}/3 = 0.5 \gamma_{k}$ is substituted into Eqs. (19a-c). Here the same characteristic length parameter $\lambda^{-1}$ as in Eqs. (40a-c) is used; the correspondence between the pp $(L_x, L_y, L_z)$ and the cube of size $L$ is given by the equality $V = L_x L_y L_z = L^3 = \lambda^{-3} l^3$.

To compare the obtained kinetic curves with the corresponding Cahn kinetics, we substitute the above $\omega^{(c)}$ value into the Cahn VF equation. In view of the equalities $\omega_{k}^{(c)}/t = (3 \lambda \gamma_{k})(2u) = 3 \gamma_{k} \bar{\tau}$, this equation is as follows:

$$Q_c(\tau) = \exp\left\{-3 \gamma_{k} \bar{\tau} \int_{0}^{1} \left[1 - e^{-\gamma_{k} \bar{\tau}(1-3\lambda^2+2\lambda^{-1})} \right] d\lambda\right\}$$ (66)

One obtains $\gamma_{1} = 0.736$, $\bar{\tau}_{1}^{(c)} = 1.104$ and $\gamma_{2} = 0.426$, $\bar{\tau}_{2}^{(c)} = 0.639$ for $k = 1$ and 2, respectively.

The normal distribution

$$f_n(l) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(l-\mu)^2}{2\sigma^2}}$$ (67)
is useful to study the change in the TK depending on the distribution width $\sigma$. One obtains $\gamma_n = 0.958$, $\gamma_n = 1.437$ and $\gamma_n = 0.858$, $\gamma_n = 1.287$ for $\sigma = 0.15$ and $0.3$, respectively; Eq. (66) holds with the replacement $\gamma_k \rightarrow \gamma_n$. It was put here.

Finally, the uniform distribution $f_c(L) = 1/2\bar{L}$ on the segment $[0, 2\bar{L}] = [0, 2\lambda^{-1}]$ with $\bar{L} = \lambda^{-1}$ is of interest as the extreme case of a wide distribution; $f_c(L) = 1/2$. As is mentioned above, the grain size distribution resulting from continuous nucleation and growth is wide and close to the uniform one. Eq. (62) has the following form in this case:

$$Q^{(c)}(\tau) = \frac{1}{4} \int_{0}^{2} Q_c(\bar{\alpha}, \bar{\tau}^{\gamma} \tau, \bar{\tau}) \, d\tau$$

(68)

Applying Eq. (65) with $f_c(L)$ instead of $g^{(k)}_k(L)$ and with integration up to 2, one obtains $\gamma_u = 2/3$, $\omega_u^{(c)} = 2\lambda$, $c_u^{(c)} = 1$, $c = 1/3$, and $2\omega_u^{(c)}ut = 2(2\lambda ut) = 2\bar{\tau}$ for the corresponding Cahn equation.

Figs. 11a-c show the kinetic curves for these four distributions in comparison with other characteristic curves for $\bar{\alpha}_s = 0.1$ and $10^3$. The first common feature of these figures is that the TK in the system of size-distributed cubes is slower than in the corresponding regular cubic structure ($L = \lambda^{-1}$, $\tau = \bar{\tau}$, and $\alpha_s = \bar{\alpha}_s$); this is the same phenomenon as in the above case of the ensemble of width-distributed plates, Fig. 1b, and random planes, Fig. 3b. In the case of normal distribution, Fig. 11c, the kinetic curve approaches that for the regular structure when the distribution width $\sigma$ decreases, as it must.

The second common feature is that the Cahn model equation underestimates the obtained kinetics, which agrees with previous studies [42, 46]. As in Fig. 9, here the exact Cahn equation instead of the MFA one is employed. However, the accuracy correction with the use of Fig. 5d does not change the relative positions of the mentioned curves at $\bar{\alpha}_s = 0.1$; this issue is absent at large $\bar{\alpha}_s$ s. It can be seen that the degree of this underestimation is different for different distributions; it is minimal for the function $g^{(k)}_k(L)$ and maximal for the normal distribution. On the other hand, Eq. (37) for the (a)-structure of pp-s corresponding to the given cubic structure overestimates the obtained TK, despite the fact that both structures have the same volume distribution of structural elements. The difference between the (a)-structure curve and Cahn’s one is due to the fact that $\gamma_i < 1$, i.e. different $\omega$-values; the given-model curve is between these two.

Fig. 11b shows the same curves as Fig. 11a, but for the function $g^{(k)}_k(L)$ corresponding to the second-order Erlang law. Accordingly, kinetics is slower here, than in the previous case, and
the curves move further away from the regular-structure graph. This also applies to the curve for the (d)-structure of pp-s (Fig. 6d) which is calculated here for Erlang’s distribution, as well as the (a)-structure curve. Finally, kinetic curves for the uniform distribution are shown in Fig. 11c. In the cases of normal and uniform distributions, Cahn’s equation noticeably underestimates the TK.

Fig. 12 shows the double-logarithmic VF plots (for $\bar{x} = 10^4$) usually employed by experimentalists for the TK analysis. While the positions of all curves in Fig. 12 (except for the BS-limit line) depend on the $\omega^{(c)}$ value (they go down with a decrease in $\omega^{(c)}$), their slope does not change; just the latter is important here. Therefore, only the Cahn curve for the $g_2^{(1)}(l)$ distribution as the lowest one and only the KJMA line for the regular ($\delta$ -distributed) cubic structure as the highest one are shown. At the early stage, each curve coincides with the corresponding KJMA line. Further, they diverge; simultaneously, the curves for cubic structures deviate from the Cahn-curve direction. In addition, the curves for $\delta$ -shaped and uniform distributions end in a pronounced steep bend, which leads to a sharp increase in the Avrami exponent [42, 47]. In the case of small $\bar{x}$ s, the Avrami exponent value is about that for the KJMA kinetics, $n = 4$. On the whole, the picture is the same as in the case of spherical geometry of grains [42].

6. Conclusions

1. A VF equation for an ensemble of width-distributed plates is derived using a VF equation for the surface-nucleated transformation of a single infinite plate. The TK of the ensemble of width-distributed plates is slowed relatively the TK of the ensemble of identical plates due to the presence of plates with a large width. These ensembles can be considered as the 1D model of grain-boundary nucleated transformation in regular and random structures under the Johnson and Mehl’s assumption that a growing nucleus cannot cross grain boundaries.

2. The mean-field approximation is used to get VF equations for the ensembles of an infinite number of parallel planes arranged both regularly and randomly. These ensembles can be considered as the 1D model of grain-boundary nucleated transformation in regular and random structures without the above Johnson and Mehl’s constraint. For the system of randomly arranged planes with the Poisson point process of their positions, an exact solution is obtained by the CR method; comparison with the MFA solution shows a high accuracy of the latter in this case. A non-Poissonian process of planes positions is considered for the first time. The exact solution obtained for the second-order Erlang process shows that it cannot be derived by the
Cahn method, which means that the extended-volume approach is not universal and only applies to Poisson processes.

3. The results obtained for random planes are used to get the VF and grain size distribution for the grain structure of random parallelepipeds formed by three sets of random planes orthogonal to each other, which is a special Cahn model. Based on this (a)-structure, various derivative ones are constructed up to the completely uncorrelated (d)-structure which is a random packing of the same parallelepipeds; the latter may approximate a real grain structure. The TK in the (a)-structure is considerably slowed down as compared to that in the (d)-structure. Considering the TK in various intermediate structures between these two, the following rule is established: the TK accelerates, when the degree of correlation in the arrangement of parallelepipeds decreases. In this way, despite the fact that all the structures consist of the same parallelepipeds transforming in the same way, the rates of transformation are different for different packings. This is the paradox of packing suggesting that the correlation in the arrangement of grains in the general Cahn model can be responsible for the TK underestimation as applied to real grain structures. The exponential 1D-growth asymptotics of Cahn’s expression originates just from random planes and, therefore, is closely related to this correlation.

4. VF equations obtained for regularly arranged planes are used to get VF equations for cubic structures, both regular and random. Four different size distributions are employed to study the TK in a random cubic structure. The corresponding Cahn equation (with the same area of boundaries in unit volume) underestimates the TK in both regular and random structures for all the distributions considered. The degree of underestimation is different for different size distributions; it is the largest in a regular structure. These results suggest that the correlation effect in the Cahn model acts systematically to underestimate the TK, but the degree of underestimation also depends on the grain size distribution of the structure under study.

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Fig. 2. To calculating the VF in the system of an infinite number of parallel planes in the MFA; explanations are in the text.
Fig. 4. To exact calculating the VF in the system of an infinite number of random parallel planes; explanations are in the text.
Fig. 6. (a) Grain structure formed by three sets of random parallel planes orthogonal to each other and therefore consisting of random parallelepipeds. The gradual weakening of correlation in the arrangement of parallelepipeds occurs in structures (b) – (d); explanations are in the text. (d) 2D section of the random packing of parallelepipeds from Fig. (a).

Fig. 8. To calculating the function $c'(\bar{\tau})$. The transformed part of the length $L$ at time $t$ is shaded; other explanations are in the text.
Fig. 1. (a) Double-logarithmic VF plots for the surface-nucleated transformation of a plate (solid) together with the corresponding KJMA lines for bulk nucleation (dashed) at different $\alpha_s$ values shown at the curves. (b) Kinetic curves for the ensemble of width-distributed plates with the exponential (dashed) and second-order Erlang (dash-dotted) distributions versus the curves for the ensemble of identical plates (solid) with $\alpha_s = \bar{\alpha}_s$. At $\alpha_s = 10^3$, each curve is close to its own BS-limit line (dotted), Eqs. (4) and (14a, b).
Fig. 3. (a) MFA kinetic curves $X^{(pl)}(\tau)$ for the ensemble of regularly arranged planes (solid) versus the kinetic curves $X^{(pl)}(\tau)$ for the ensemble of isolated identical plates (dashed) at different $\alpha_s$ values. (b) MFA kinetic curves for regular (solid) and random (dashed) planes with the exponential distribution (the 1D Cahn model) for different $\alpha_s$ values.
Fig. 5a, b.
Fig. 5. (a) Kinetic curves $X_{(1)}(\bar{\tau})$ (dashed) and $X_{(2)}(\bar{\tau})$ (solid) for the Poisson and second-order Erlang distribution of planes, respectively, as a result of exact solution. The corresponding BS-limit lines (dotted) are given by Eqs. (14a, b). (b) MFA (dashed) versus exact (solid) kinetic curves for the P-process of planes at different $\alpha_x$ values. (c) MFA (dashed) versus exact (solid) kinetic curves for the E$_2$-process of planes. (d) MFA error for the P-process (top solid) and E$_2$-process (dashed) at different $\alpha_x$ values, as well as MFA error for the VF cubes $\Delta X_{(i)}^{(c)}(\bar{\tau})$ (bottom solid).
Fig. 7. (a) Kinetic curves $X_{\alpha}(\tau)$, $\alpha = a, b, c, d$ (solid), $b', c'$ (dashed), and $B, C$ (dash-dotted) for the structures of Fig. 6. (b) Differences between curves (c) and (c') as well as (b) and (b').
Fig. 9. Kinetic curves for the regular cubic structure (solid), the dual structure of inscribed spheres [42] (dash-dotted), and Cahn’s model (dashed) for different $\alpha_s$ values. The BS-limit line (dotted) represents Eq. (60).
Fig. 10. (a) Volume distribution $g_k(\nu)$ of parallelepipeds for $k = 1, 2, 3, \text{ and } 4$, Eq. (40b). (b) Size distribution of cubes of the same volumes, Eq. (40c).
Fig. 11a, b.
Fig. 11. Kinetic curves for the structures of size-distributed cubes (solid) with the $g_1^{(i)}(l)$ (a), $g_2^{(i)}(l)$ (b), normal with $\sigma = 0.15$ and 0.3 (c), and uniform (d) distributions. Other curves are for the following structures: regular cubic (short dash), Cahn’s model (dashed), the (a)- and (d)-structures of parallelepipeds of Fig. 6 (dash-dotted); the BS-limit line for size-distributed cubes, Eq. (64), is dotted.
Fig. 12. Double-logarithmic VF curves for the grain structures of size-distributed cubes for different distributions.