Dynamical germ-grain models with ellipsoidal shape of the grains for some particular phase transformations in Materials Science

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Abstract. A large number of engineering materials of interest are aggregate of many small crystals, called the grains of the polycrystal, which are often equiaxed. However, because of processing, the grain shape may become anisotropic; for instance, during recrystallization or phase transformations, the new grains may grow in the form of ellipsoids. Moreover, it is reasonable and it has also been found in experimental works, that the probability of a new nucleus forming very close to another one is likely to be low. From a mathematical point of view, such situation may be modelled by assuming hard-core nucleation processes.
We collect here a series of recent results on mean volume and surface densities of suitable dynamical germ-grain models with ellipsoidal shape of the grains, with the aim to provide a unified approach in modelling phase transformations of this kind.

Keywords: Birth-and-growth process, random set, point process, phase transformation

1 Introduction

Formal kinetics is frequently employed to analyze a variety of heterogenous transformations in condensed phases. The early theory developed by Johnson-Mehl[13], Avrami[1–3], and Kolmogorov[15], known as KJMA theory, has constituted the foundation of formal kinetics theories applied today. Heterogeneous transformations may be defined as those transformations in which there is a moving boundary between the transformed and untransformed region. This formalism envisages that the heterogeneous transformations may be decomposed in two stages. The first stage, the nucleation, is that in which the transformed region originates. On the other hand, the second stage, the growth stage, is that in which the transformed region grows consuming the parent matrix. The fundamental way of modelling nucleation and growth transformations is by relying on the physics of the transformations mechanisms. However, this is not always

feasible and an alternative treatment is provided by the so-called *formal or global kinetics*, that is a branch of solid-state transformations theory that deals with nucleation and growth in a phenomenological way, that is, it "prescribes" how nucleation and growth take place. Namely, a birth-and-growth (stochastic) process is a dynamic *germ-grain model* (e.g., see [7]) used to model situations in which *nuclei* (germs) are born in time and are located in space randomly, and each nucleus generates a *grain* evolving in time according with a given growth law. Since, in general, the nucleation is random in time and space, then the transformed region at any time $t > 0$ will be a random set in $\mathbb{R}^d$, that is a measurable map from a probability space to the space of closed subsets in $\mathbb{R}^d$ [7]. Denote by T_j the $\mathbb{R}_+$-valued random variable representing the *time of birth* of the j-th nucleus, and by X_j the $\mathbb{R}^d$-valued random variable representing the *spatial location* of the nucleus born at time T_j; the sequence $N = \{(T_i, X_i)\}$ is called nucleation process. Let $\Theta^t_{T_j}(X_j)$ be the grain obtained as the evolution up to time $t \geq T_j$ of the nucleus born at time T_j in X_j; then, the transformed region Θ^t at time t is given by

$$\Theta^t = \bigcup_{(T_j, X_j) \in N \,:\, T_j \leq t} \Theta^t_{T_j}(X_j), \qquad t \in \mathbb{R}_+. \tag{1}$$

The family $\{\Theta^t\}_t$ is called *birth-and-growth process*; the materials scientists denote it *microstructure* of the sample.
Since Θ^t is a random set, it gives rise to a random measure $\nu^d(\Theta^t \cap \cdot\,)$ in $\mathbb{R}^d$ for all $t > 0$, having denoted by ν^d the d-dimensional Lebesgue measure in $\mathbb{R}^d$. In particular, it is of interest to consider the *expected volume measure* $\mathbb{E}[\nu^d(\Theta^t \cap \cdot\,)]$ and its density (i.e., its Radon-Nikodym derivative), called *mean volume density of* Θ^t and denoted by V_V, provided it exists:

$$\mathbb{E}[\nu^d(\Theta^t \cap A)] = \int_A V_V(t, x)\mathrm{d}x \qquad \forall A \in \mathcal{B}_{\mathbb{R}^d}, \tag{2}$$

where $\mathcal{B}_{\mathbb{R}^d}$ is the Borel σ-algebra of $\mathbb{R}^d$. Whenever $V_V(t)$ is independent of x (e.g., under assumptions of homogeneous nucleation and growth), it is called *volume fraction at time* t. A related quantity is the *mean extended volume density* at time t, denoted by $V_E(t, \cdot)$ and defined as the density of the *mean extended volume measure* at time t on $\mathbb{R}^d$:

$$\mathbb{E}[\sum_{j : T_j \leq t} \nu^d(\Theta^t_{T_j}(X_j) \cap A)] = \int_A V_E(t, x)\mathrm{d}x, \qquad \forall A \in \mathcal{B}_{\mathbb{R}^d}.$$

The following further quantities are defined in a similar way: $S_V(t, \cdot)$, the *mean surface density* at time t, defined to be the density of the *mean surface measure* at time t: $\mathbb{E}[\mathcal{H}^{d-1}(\partial\Theta \cap \cdot\,)]$; and $S_E(t, \cdot)$, the *mean extended surface density* at time t, defined to be the density of the *mean extended surface measure* at time t: $\mathbb{E}[\sum_{j : T_j \leq t} \mathcal{H}^{d-1}(\partial\Theta^t_{T_j}(X_j) \cap \cdot\,)]$. Here $\mathcal{H}^{d-1}$ is the $n-1$-dimensional Hausdorff measure, while ∂A is the topological boundary of a set $A \subset \mathbb{R}^d$. In other words, the mean extended volume and surface measures represent the mean of the sum

of the volume measures and of the surface measures of the grains which are born and grown until time t, supposed *free to grow*, ignoring overlapping. (See also [21].)
Of course, different kinds of nucleation and growth models gives rise to different kinds of processes $\{\Theta^t\}_t$. Thus, let $\{\Theta^t\}_t$ be a birth-and-growth process modelling a particular phase transformation of interest. A problem is to find out explicit formulas for V_V and the related quantities above mentioned, associated to Θ^t.
A considerable number of engineering materials are polycrystal: an aggregate of many crystals with size usually below 100μm. Those small crystals are called the grains of the polycrystal, and are often equiaxed; however, because of processing, the grain shape may become anisotropic. For instance, during recrystallization or phase transformations, the new grains may grow in the form of ellipsoids. Indeed, even if the assumption of spherical growth is standard and allows to get more explicit formulas, new regions do not always grow as spheres (e.g., see [11, 24, 25]. Bradley *et al.* demonstrated in a series of papers [4–6] that a grain boundary nucleated ferrite allotriomorph is best described by an oblate ellipsoid. The reason why these regions grow with ellipsoidal shape is that the growth on the grain boundary plane is faster than the thickening into the austenite. Actually, regarding ellipsoidal grains, one has two related issues. One is the growth of ellipsoidal grains with nuclei located randomly in space, allowed to overlap each other or not. We also mention that when a polycrystal is deformed by cold rolling, the resulting pattern may be modelled as a random union of ellipsoids with a fixed orientation (the major axis is in the direction of the rolling). The other issue is the growth of ellipsoidal grains with nuclei located on random parallel planes. This occurs for example in recrystallization processes after heavy rolling: to a first approximation, one may consider that these anisotropic grains may be approximated by random parallel planes; subsequently a new nucleation takes place on such planes.
Finally, we also mention that it is reasonable and it has also been found in experimental works, that the probability of a new nucleus forming very close to another one is likely to be low. Therefore, one might suppose that in some cases there is effectively an "exclusion radius" around each nucleus so that within that radius nucleation cannot occur. From a mathematical point of view, such situation may be modelled by assuming *hard-core nucleation processes*.

The three different birth-and-growth processes (ellipsoidal growth with nuclei randomly located in space, on parallel planes, and having an exclusion zone around each nucleus) modelling the real situations above mentioned have been recently faced by the authors in a series of papers (see in particular [28, 17, 26]). Here we propose a survey of them by collecting and specializing the most relevant results concerning the case of ellipsoidal grains.

2 Preliminaries and notation

In this section we fix basic notation and we summirize some preliminary results useful for the sequel.

Throughout the paper we work in the Euclidean space $\mathbb{R}^d$, $d \geq 2$; $\mathcal{H}^n$ is the n-dimensional Hausdorff measure, $\mathcal{B}_{\mathbb{R}^d}$ is the Borel σ-algebra of $\mathbb{R}^d$, and ν^d denotes the usual d-dimensional Lebesgue volume measure (which coincides with $\mathcal{H}^d$ in $\mathbb{R}^d$). Given a subset A of $\mathbb{R}^d$, A^c denotes the complemetary set of A, whereas $\partial A := \mathrm{cl}A \setminus \mathrm{int}A$ its topological boundary. For $r \geq 0$ and $x \in \mathbb{R}^d$, $B_r(x)$ is the closed ball with centre x and radius r; finally, for every integer $n > 0$, b_n denotes the volume of the unit ball in $\mathbb{R}^n$, while S^{d-1} the unit sphere in $\mathbb{R}^d$.

2.1 Point process and germ-grain model

A nucleation process is said to be *site-saturated* if the nucleation rate is so fast at the beginning of the transformation that the available nucleation sites are saturated early in the transformation. Therefore, site-saturation essentially signifies that all nuclei are already present at the time origin and no nuclei form later in the transformation. Otherwise we say that the nucelation process is *time-dependent*. Site-saturated and time-dependent nucleation processes can be modelled by means of *(marked) point processes*. We give here some basic concepts and definitions useful in what follows, without entering into the details of the mathematical theory of point processes (see [8, 9] for an exhaustive treatment).

A point process in $\mathbb{R}^d$, say $\widetilde{\Phi}$, is a locally finite collection $\{X_i\}_{i\in\mathbb{N}}$ of random points; more formally $\widetilde{\Phi}$ is a random counting measure, that is a measurable map from a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ into the space of locally finite counting measures on $\mathbb{R}^d$. The measure $\widetilde{\Lambda}(A) := \mathbb{E}[\widetilde{\Phi}(A)]$ on $\mathcal{B}_{\mathbb{R}^d}$ is called *intensity measure* of $\widetilde{\Phi}$. We also remind that $\widetilde{\Phi}$ is called *Poisson process* whenever has independent increments and it is such that $\mathbb{P}(\widetilde{\Phi}(A) = n) = \frac{\widetilde{\Lambda}(A)^n}{n!} e^{-\widetilde{\Lambda}(A)}$ for all $A \in \mathcal{B}_{\mathbb{R}^d}$, $n \in \{0, 1, 2, \ldots\}$.

A *Marked point process* in $\mathbb{R}^d$ with *marks* in a complete and separable metric space $\mathbf{K}$, is a collection $\Phi = \{(X_i, K_i)\}_{i\in\mathbb{N}}$ of random points X_i in $\mathbb{R}^d$, each one associated with a mark $K_i \in \mathbf{K}$, with the property that the unmarked process $\{\widetilde{\Phi}(B) : B \in \mathcal{B}_{\mathbb{R}^d}\} := \{\Phi(B \times \mathbf{K}) : B \in \mathcal{B}_{\mathbb{R}^d}\}$ is a point process in $\mathbb{R}^d$. The intensity measure of Φ, say Λ, is a σ-finite measure on $\mathcal{B}_{\mathbb{R}^d \times \mathbf{K}}$ defined as $\Lambda(B \times L) := \mathbb{E}[\Phi(B \times L)]$. It is worth recalling that a marked Poisson point process can be seen as a Poisson point process on the product space $\mathbb{R}^d \times \mathbf{K}$; the assumption of Poissonian nucleation enables to get more explicit results when dealing with birth-and-growth processes.

Notice that a point process $N = \{X_i\}$ in $\mathbb{R}^d$ may be taken as model for a site-saturated nucleation process, whereas a marked point process $N = \{(T_i, X_i)\}$ in $\mathbb{R}_+$ with marks in $\mathbb{R}^d$ may be taken as model for a time-dependent nucleation process. In this latter case, $\Lambda([0, t] \times B)$ gives the mean number of nuclei which are born in $B \in \mathcal{B}_{\mathbb{R}^d}$ during the time interval $[0, t]$.

A *random closed set* Θ in $\mathbb{R}^d$ is a measurable map $\Theta : (\Omega, \mathcal{F}, \mathbb{P}) \longrightarrow (\mathbb{F}, \sigma_{\mathbb{F}})$, where $\mathbb{F}$ denotes the class of the closed subsets in $\mathbb{R}^d$, and $\sigma_{\mathbb{F}}$ is the σ-algebra generated by the so called *Fell topology*, or *hit-or-miss topology* (e.g., see [7]). Any random closed set in $\mathbb{R}^d$ given by a random union of compact random sets (*particles*) can be represented as *germ-grain model*. This latter is decribed by a suitable marked point process Φ in $\mathbb{R}^d$ with marks in $\mathcal{K}^d$, the space of compact subsets of $\mathbb{R}^d$. Namely, a germ-grain model is a random set of the type

$$\Theta = \bigcup_{(X_j, Z_j) \in \Phi} X_j + Z_j, \tag{3}$$

where $\Phi = \{(X_j, Z_j)\}_{j \in \mathbb{N}}$ is a *marked point process* in $\mathbb{R}^d$ with marks in $\mathbf{K} := \mathcal{K}^d$ so that Z_j is a compact random set containing the origin.
It is then clear why the family $\{\Theta^t\}_{t \in \mathbb{R}_+}$ with Θ^t defined as in (1) where the role of $X_j + Z_j$ and of Φ in (7) are played by $\Theta^t_{T_j}(X_j)$ and by N, respectively, is also called *dynamical germ-grain model*.

Remark 1. We point out, that, in dependence on the growth model, the nucleation point process N has to be chosen in order to well describes the process $\{\Theta^t\}_t$ accordingly. For instance a point process $N = \{(T_i, (X_i, G_i)\}$ in $\mathbb{R}_+$ with marks in $\mathbb{R}^d \times \mathbb{R}_+$ may be taken to model the case of time dependent nucleation and spherical growth model with random constant velocity of each nucleus (e.g., see [22] for further insights):

$$\Theta^t = \bigcup_{(T_i, X_i, G_i) \in N \,:\, T_i \leq t} B_{G_i(t-T_i)}(X_i) \qquad \forall t \geq 0.$$

2.2 The ellipsoidal growth model

Dealing with birth-and-growth processes, beside the definition of a suitable nucleation process, one has to define also a growth model. Here we shall consider the following *ellipsoidal growth model* in $\mathbb{R}^3$:
Let us fix $a = (a_1, a_2, a_3) \in \mathbb{R}^3_+$; we denote by

$$\mathcal{E}_0(a) := \left\{ (x_1, x_2, x_3) \in \mathbb{R}^3 \,:\, \frac{x_1^2}{a_1^2} + \frac{x_2^2}{a_2^2} + \frac{x_3^2}{a_3^2} \leq 1 \right\}$$

the ellipsoid centred in the origin with semiaxes a_1, a_2 and a_3 aligned with the axes $\hat{x}$, $\hat{y}$ and $\hat{z}$, respectively. For any $\phi \in SO(3)$, where $SO(3)$ is the rotation group in $\mathbb{R}^3$,we denote by $\mathcal{E}_0(a; \phi)$ the ellipsoid $\mathcal{E}_0(a)$ rotated according to ϕ.
We assume that the grains grow with ellipsoidal shape with constant rate $G > 0$, that is at any time t the grain born at point x at time s and grown up to time t, is given by an ellipsoid centred at x with semiaxes of length $a_1 G(t-s)$, $a_2 G(t-s)$ and $a_3 G(t-s)$ respectively, randomly orientated into the space. By random orientation we mean that the direction ϕ of the a_1-semiaxis of the ellipsoid is random, accordingly with a given probability distribution Q on $SO(3)$, independent on the spatial location and on the birth time of the corresponding

nucleus. Hence, denoted by $\Theta_s^t(x,\phi)$ the grain born in x at time s and grown with orientation ϕ until time t, we have

$$\Theta_s^t(x,\phi) = x + \mathcal{E}_0(G(t-s)a;\phi) = x + G(t-s)\mathcal{E}_0(a;\phi) \qquad \forall s \le t, \tag{4}$$

Note that for any time t the ratio between the axes of the grain remains constant (that is during the transformation only the size of the grain is varying, not the shape). This models for instance the transformed phase deformed after rolling. Note also that the case of spherical growth with constant velocity follows as particular case by putting $a_1 = a_2 = a_3 = 1$; of course ϕ does not make any role, $\mathcal{E}_0 = \mathcal{E}_0(\phi) = B_1(0)\ \forall \phi \in \mathbf{S}^2$, and $\Theta_s^t(x) = B_{G(t-s)}(x)$.

2.3 The causal cone notion

It is well known and it easily follows by a direct application of Fubini theorem in (2) that

$$V_V(t,x) = \mathbb{P}(x \in \Theta^t).$$

The so-called *causal cone* of a point x at time t, denoted here by $\mathcal{C}(t,x)$, plays a fundamental role in evaluating $V_V(t,x)$. It is defined as the *region* (i.e., the subset of the space where the nucleation process N takes values) in which at least one nucleation event has to take place in order to cover the point x at time t. Namely, the following equivalence between events holds:

$$\{x \in \Theta^t\} \iff \{N(\mathcal{C}(t,x)) > 0\}.$$

As a consequence, if N is a Poisson process with intensity measure Λ, then

$$V_V(t,x) = 1 - \mathbb{P}(N(\mathcal{C}(t,x)) = 0) = 1 - e^{-\Lambda(\mathcal{C}(t,x))}. \tag{5}$$

We already pointed out that different birth-and-growth processes are driven by different nucleation processes. Therefore if N takes value in a space E, then the associated causal cone will be a subspace of E; for instance, with reference to the example given in Remark 1, $E = \mathbb{R}_+ \times \mathbb{R}^d \times \mathbb{R}_+$ and

$$\mathcal{C}(t,x) := \{(s,y,g) \in E\ :\ s \in [0,t],\ x \in B_{g(t-s)}(y)\}.$$

In the simpler case in which the volocity is constant equal to G for each grain, then $E = \mathbb{R}_+ \times \mathbb{R}^d$, and $\mathcal{C}(t,x) := \{(s,y) \in E\ :\ s \in [0,t],\ x \in B_{G(t-s)}(y)\}$. Note that $x \in B_R(y)$ if and only if $y \in B_R(x)$, and that in the subcase of site-saturation $E = \mathbb{R}^d$ and $\mathcal{C}(t,x) = B_{Gt}(x)$.

3 Three different models with ellipsoidal grains

Throughout the paper we shall consider birth-and-growth processes in $\mathbb{R}^3$ for applicative reasons, but all our argumentation applies to any dimension $d \ge 2$.

3.1 Ellipsoidal growth with space nucleation

Let us consider the birth-and-growth process in $\mathbb{R}^3$ driven by a time dependent Poissonian nucleation process in space, and growth model defined as in Section 2.2.

Hence, let the nucleation process N be a Poisson point process in $E = \mathbb{R}_+ \times \mathbb{R}^3 \times SO(3)$ with intensity measure

$$\Lambda(\mathrm{d}(s, x, \phi)) = g(s)f(x)\mathrm{d}s\mathrm{d}xQ(\mathrm{d}\phi), \tag{6}$$

where g and f are non-negative locally integrable functions on $\mathbb{R}_+$ and $\mathbb{R}^3$, respectively, while Q is a probability measure on $SO(3)$.
The intensity measure of the type (6) models the fact that the location and the orientation of each grain are independent each other and independent of the corresponding time birth. We remind that $\Lambda([T_1, T_2] \times A \times B)$ is the mean number of nuclei which are born in A during the time interval $[T_1, T_2]$, and whose associated ellipsoids have orientation in $B \subseteq SO(3)$. The subcase of constant rate I is given by taking $g(t) \equiv I > 0$. Analogously, the subcase of homogenous spatial location of the nuclei is modelled by choosing $f(x) \equiv c > 0$. A fixed orientation $\bar{\phi} \in SO(3)$ is described by choosing $Q(\mathrm{d}\phi) = \delta_{\bar{\phi}}(\phi)\mathrm{d}\phi$, where $\delta_{\bar{\phi}}(\phi)$ is the classical Dirac-delta function in $\bar{\phi}$.
Then the transformed region Θ^t at time t is the random closed set

$$\Theta^t := \bigcup_{(s_n, x_n, \phi_n) \in N} \Theta^t_{s_n}(x_n, \phi_n), \tag{7}$$

with $\Theta^t_{s_n}(x_n, \phi_n)$ as in (4) for any $s_n \leq t$, and the empty set for any $s_n > t$; therefore

$$\begin{aligned} \mathcal{C}(t, x) &:= \{(s, y, \phi) \in [0, t] \times \mathbb{R}^3 \times SO(3) \,:\, x \in \Theta^t_s(y, \phi)\} \\ &= \{(s, y, \phi) \in [0, t] \times \mathbb{R}^3 \times SO(3) \,:\, y \in \Theta^t_s(x, \phi)\}, \end{aligned} \tag{8}$$

where the latter equation follows by the central symmetry of the grains.
It is easy to show (e.g., see [28]) that

$$V_E(t, x) = \Lambda(\mathcal{C}(t, x)), \tag{9}$$

and so by (5) and (8):

$$V_V(t, x) = 1 - \exp\Big\{ - \int_0^t g(s)\Big(\int_{SO(3)} \int_{\Theta^t_s(x,\phi)} f(y)\mathrm{d}yQ(\mathrm{d}\phi)\Big)\mathrm{d}s\Big\}.$$

The computation of the above integral might be difficult whenever f is not constant. In addition to the situations in which nuclei are located uniformly within the specimen (case f constant), it is also of interest to study situations in which nuclei vary along a preferential direction. In [28, Appendix] a generalization of

the so-called *mean value property for harmonic function* has been proved; in the special case of ellipsoids in $\mathbb{R}^3$ this implies that

$$\int_{x+\mathcal{E}_0(a)} h(y)\mathrm{d}y = h(x)\frac{4}{3}\pi a_1 a_2 a_3$$

for any $h \in C^2(\mathbb{R}^3, \mathbb{R})$ such that $\sum_i a_i^2 \partial_i^2 h = 0$. Therefore, if we assume f varying along a preferential direction, that is of the type

$$f(x) = \sum_{i=1}^{3} p_i x_i + q, \tag{10}$$

with $p = (p_1, p_2, p_3) \in \mathbb{R}^3$, and $q \in \mathbb{R}$ such that $f(x) \geq 0$ for any x in the considered observation window, then the associated volume density $V_V(t, x)$ simplifies as

$$V_V(t, x) = 1 - \exp\Big\{ - f(x)\frac{4}{3}\pi G^3 a_1 a_2 a_3 \int_0^t g(s)(t-s)^3 \mathrm{d}s \Big\}. \tag{11}$$

Fig. 1 depicts a particular case of Eq. (11) in which $f(x) = 1$ and the nucleation is site-saturated. (Site-saturation is modelled by putting $g(s) = \delta_0(s)$, the Dirac delta function at 0, so that $\int_0^t g(s)(t-s)^3 \mathrm{d}s = t^3$ in (11).) Fig. 1 shows the mean volume density as a function of dimensionless time for the growth of regions when those regions are: a ball and oblate ellipsoids of different relations of longer to shorter axis.

Before passing to consider the mean surface densities S_V and S_E, let us recall the notion of *support function of a convex body.*

Definition 1. *Let C be a convex body in $\mathbb{R}^d$ (that is a compact and convex set containing 0 in its interior). The support function h_C of C is the function so defined:*

$$h_C(v) := \sup_{x \in C} x \cdot v, \quad v \in \mathbb{R}^d,$$

We point out that, by denoting $\widetilde{a}_M := \max\{a_1, a_2, a_3\}$ and $\widetilde{a}_m := \min\{a_1, a_2, a_3\}$, the support fuction of $\mathcal{E}_0(a; \phi)$ is such that

$$\widetilde{a}_m \leq h_{\mathcal{E}_0(a;\phi)}(y) \leq \widetilde{a}_M \qquad \forall y \in \mathbb{R}^d. \tag{12}$$

In [28] the mean surface density has been studied as well; we may summarize the main results in the following

Proposition 1. *Let Θ^t be defined as in* (7)*, with N having intensity measure Λ as in* (6)*. Then*

$$S_V(t, x) = (1 - V_V(t, x))S_E(t, x), \tag{13}$$

with

$$S_E(t, x) = \int_0^t g(s) \int_{SO(3)} \int_{\partial\Theta_s^t(x,\phi))} f(y)\mathcal{H}^2(\mathrm{d}y)Q(\mathrm{d}\phi)\mathrm{d}s. \tag{14}$$

Moreover,

$$\frac{\partial}{\partial t}V_V(t,x) = (1-V_V(t,x))G\int_0^t g(s)\int_{SO(3)}\int_{\partial\Theta_s^t(x,\phi)} f(y)h_{\mathcal{E}_0(a;\phi)}(\nu_{\Theta_s^t(x,\phi)}(y))\mathcal{H}^2(\mathrm{d}y)Q(\mathrm{d}\phi)\mathrm{d}s, \tag{15}$$

where $h_{\mathcal{E}_0(a;\phi)}$ is the support function of the convex body $\mathcal{E}_0(a;\phi)$, whereas $\nu_{\Theta_s^t(x,\phi)}(y)$ is the outer normal to $\Theta_s^t(x,\phi)$ at y.

Remark 2. In the spherical growth case, that is $\mathcal{E}_0(a;\phi) = B_1(0)$, it is well known (e.g., see [21]) that :

$$S_V(t,x) = \frac{1}{G}\frac{\partial}{\partial t}V_V(t,x). \tag{16}$$

This is in accordance with the above proposition by taking into acocunt that $h_{B_1(0)}(y) = 1$ for any $y \in \mathbb{R}^d$, and that Q is a probability measure in $SO(3)$. In the general ellipsoidal growth model, Eq. (16) is not true any more. Actually, by (12), (14) and (15) we have

$$(1 - V_V(t,x))G\widetilde{a}_m S_E(t,x) \le \frac{\partial}{\partial t}V_V(t,x) \le (1 - V_V(t,x))G\widetilde{a}_M S_E(t,x),$$

and so by (13)

$$\frac{1}{G\widetilde{a}_M}\frac{\partial}{\partial t}V_V(t,x) \le S_V(t,x) \le \frac{1}{G\widetilde{a}_m}\frac{\partial}{\partial t}V_V(t,x).$$

As a further generalization, one might consider the case of random velocity of the grains, as well. As a matter of fact, in [12] the authors reviewed their experimental measures of growth velocities of individual grains obtained by neutron and 3- dimensional synchrotron X-ray methods, and they concluded that there is compelling evidence to support that "every single grain has its own kinetics different from the other grains". In accordance to Remark 1, to model the fact that each grain has its own random growth rate, it is sufficient to add a further mark to the nucleation point process N. Namely, let N be now a Poisson point process in $E = \mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}_+ \times SO(3)$, so that any point $(s_i, x_i, \xi_i, \phi_i) \in N$ represents the nucleus which is born at time s_i at location x_i from which an ellipsoid with orientation ϕ_i and velocity ξ_i develops; that is the associated grain is given by

$$\Theta_{s_i}^t(x_i, \xi_i, \phi_i) = x_i + \xi_i(t-s)\mathcal{E}_0(a, \phi_i).$$

Of course the velocity ξ_i might be dependent on the position, and/or on the orientation ϕ_i, and/or on the birth time s_i; this would lead to formulas difficult to explicitate. Hence, let us assume independent growth velocity; this means that the random variable $\{\xi_i\}_i$ have identical probability distribution, say Q_1 on $\mathbb{R}_+$. In particular let us assume that the intensity measure Λ of N is of the type

$$\Lambda(\mathrm{d}(s,x,\phi)) = g(s)f(x)\mathrm{d}s\mathrm{d}xQ_1(\mathrm{d}\xi)Q_2(\mathrm{d}\phi),$$

with f as in (10), and Q_1 and Q_2 probability measures on $\mathbb{R}_+$ and $SO(3)$, respectivley. Moreover let $\widetilde{G} := \int_{\mathbb{R}_+} \xi^3 Q_1(\mathrm{d}\xi) < \infty$. By proceeding along the same lines that led to (11), one easily get

$$V_V(x,t) = 1 - \exp\Big\{ - f(x)\frac{4}{3}\pi\widetilde{G}a_1a_2a_3 \int_0^t g(s)(t-s)^3\mathrm{d}s\Big\}.$$

Now (11) follows here as particular case. Further generalization may be obtained by arguing similarly to what was done in [27], where the case of random spherical growth has been investigated.

3.2 Ellipsoidal growth with nucleation on parallel planes

As mentioned in the Introduction, to a first approximation in modelling recrystallization after heavy rolling, one may consider nucleation of ellipsoids on random parallel planes. More precisely, let us consider nucleation on random parallel planes with outer normal vector $w = (0,0,1) \in S^2$, and ellipsoidal growth, as in Section 2.2, but with a fixed orientation such that the major axis is parallel to the plane (in order to model major elongation in the direction of the rolling).

Let us denote by $B(u) := \{x \in \mathbb{R}^3 : x_3 = u\}$ the plane with outer normal vector $w = (0,0,1)$ and distance $|u|$ from the origin, and by $\delta_{B(u)}(y)$ the *delta function* associated to $B(u)$ (which can be seen as a generalization to the well-known delta-function δ_{x_0} associated to a point $x_0 \in \mathbb{R}^d$), so that, formally,

$$\int_A \delta_{B(u)}(y)\mathrm{d}y := \mathcal{H}^2(B(u) \cap A) \qquad \forall A \in \mathcal{B}_{\mathbb{R}^3}.$$

We also denote by $N_u = \{(s_i, x_i)\}_i$ the Poisson point process on $B(u)$ with intensity measure

$$\Lambda_u(\mathrm{d}(t,x)) = g(t)f(x)\delta_{B(u)}(x)\mathrm{d}t\mathrm{d}x$$

with f as in (10). Note that it is zero the probability of having nucleation in $B(u)^c$. Then, the transformed region $\Theta^{t,u}$ at time t associated to N_u is given by

$$\Theta^{t,u} := \bigcup_{(s_i,x_i)\in N_u} \Theta^t_{s_i}(x_i), \tag{17}$$

with $\Theta^t_{s_i}(x_i) = x_i + G(t-s_i)\mathcal{E}_0(a)$.

To model the nucleation on random parallel planes, let us introduce the point process $\Xi = \{D_j\}_j$ on the positive x_3-semiaxis, representing the random distances from the origin of the planes $B_1 = B(D_1)$, $B_2 = B(D_2), \ldots$, respectively. We shall consider the transformed region, say Θ^t_K, due to the nucleation on the random planes contained in $\mathbb{R}^2 \times [0,K]$. Thus, denoted by $\Xi_{|K} := \Xi \cap [0,K]$ the restriction of Ξ to $[0,K]$, the associated transformed region at time t will be

$$\Theta^t_K = \bigcup_{D_i \in \Xi_{|K}} \Theta^{t,D_i}, \qquad \forall t > 0, \tag{18}$$

where, for any realization $D_i = u_i$, Θ^{t,u_i} is defined as in (17).
Note that whenever Ξ is a Poisson point process with intensity $h = h(u)$, then the mean number of planes in $[0, K]$ is given by $\int_0^K h(u)\mathrm{d}u$.
By following the same approach used in [17], the following explicit expression for V_V can be proved:

Theorem 1. *[28, Theorem 10] Let $\Xi = \{D_j\}_j$ be a Poisson point process with intensity $h = h(u)$. Then, for any $t > 0$, the mean volume density $V_V(t, x)$ in x at time t of the transformed region Θ_K^t at time t, defined as in* (18) *is equal to*

$$V_V(t.x) = 1 - \exp\Big\{ - \int_0^K V_V^u(t, x)h(u)\mathrm{d}u\Big\},$$

where

$$V_V^u(t, x) = 1 - \exp\Big\{ - f((x_1, x_2, u))\pi a_1 a_2 \int_0^{t-\frac{|u-x_3|}{Ga_3}} g(s)\Big(G^2(t-s)^2 - \frac{(u-x_3)^2}{a_3^2}\Big)\mathrm{d}s\mathbf{1}_{[0,Gta_3]}(|u-x_3|)\Big\}.$$

We point out that the assumption (10) on f is crucial in order to get the above explicit tractable expression for V_V. Such formula is further simplified in the particular cases of *constant nucleation rate* $g(s) \equiv I$, and of *site-saturation* (see [28]). Computer simulation results compared with the corresponding analytical formulas are provided in [19].

3.3 Nucleation with exclusion zone around each nucleus

As mentioned in the Introduction, it has been found in experimental work that the probability of a new nucleus forming very close to another one is likely to be low. For instance, Sudbrack *et al.* experimentally proved in [23] the existence of exclusion zones in the solid-state: although uniform, the nucleation process was not in agreement with a Poisson point process. In their work, they experimentally determined the so-called *pair correlation function* of the process (e.g., see [7]) by means of planar sections, and inferred that, actually, it was consistent with each nuclei having an exclusion zone around it in their Ni-Cr-Al superalloy. Hence, as a first approximation, one may suppose that in some cases there is effectively an "exclusion zone" around each nucleus where nucleation cannot occur. In order to model a such situation, one might assume a nucleation process of the *hard-core* type. A hard-core point process is characterized by the fact that its points have a prescribed minimum distance each other. The Strauss hard-core process and the Matérn point process of type I are the most popular point processes modelling the hard-core property between points, and both of them are defined in terms of an underlying Poisson point process (e.g., see [7] for a classical reference). Roughly speaking, the Matérn I hard-core point process is obtained by deleting every point in the Poisson point process with its nearest neighbor closer than a given hard-core distance. In the classical definition, the underlying

Poisson point process is assumed to be homogeneous, but further generalizations to the inhomogeneous case and to different thinning rules are also available in the literature. The Strauss hard-core point process is a particular Gibbs point process, that is a point process whose probability distribution has density with respect to a unit rate Poisson process (e.g., see [10]); the form of such density models the hard-core property.
In the recent paper [26], the authors investigated the exclusion zone in solid-state by means of 2D simulation studies employing four different hard-core point processes: Matérn I, Matérn II, Strauss hard-core and Sequential. With reference to the above mentioned work by Sudbrack *et al.* [23], Fig. 2 below shows the comparison between the pair correlation function of the experimental work in [23] and that one of a simulated Strauss hard-core process.

We recall here in simple words the notion of Strauss and Matérn I hard-core point process with minimal interpoint distance R in $\mathbb{R}^d$. We refer to classical literature for more general definitions.
Let Z be a Poisson point process in $\mathbb{R}^d$ with finite intensity measure $\Lambda(\mathrm{d}x) = f(x)\mathrm{d}x$ and probability law distribution P_Z on the space $(S, \mathcal{S})$ of locally finite sequences of points in $\mathbb{R}^d$. A finite point process Φ in $\mathbb{R}^d$ is said to be a *point process with density p with respect to Z* if its distribution P_X on $(S, \mathcal{S})$ is absolutely continuous with respect to P_Z with density p. Without loss of generality, p may be written as

$$p(\mathbf{x}) = \alpha q(\mathbf{x}), \quad \mathbf{x} \in S, \tag{19}$$

where $q : S \to \mathbb{R}_+$ is an integrable function, said *interaction function*, and $\alpha > 0$ is a *normalizing constant*. We remind that in general the normalizing constant α is not explicitly computable.

Definition 2. *A point process Φ_{Str} with density p with respect to Z as in* (19)*, is called Strauss hard-core process if the interaction function q is of the type*

$$q(\mathbf{x}) = \mathbf{1}_{\{\|x_i - x_j\| > R,\ \forall x_i, x_j \in \mathbf{x}\}}(\mathbf{x}), \qquad \mathbf{x} \in S.$$

Definition 3. *A point process Φ_{Mat} is called Matérn I hard-core point process with underlying Poisson point process Z if $\Phi_{Mat} := \{x \in Z : Z \setminus \{x\} \cap B_R(x) = \emptyset\}$.*

Remark 3. Note that both the processes Φ_{Str} and Φ_{Mat} defined above may be taken to model centres of non-overlapping balls with radius $R/2$. It is intuitive that the above definitions may be generalized in order to model random patterns of non-overlapping grains, and so in particular non-overlapping ellipsoids. About generalizations in this direction, we refer to [14, 16] and to [18] for generalizations of the Matérn hard-core and of the Strauss hard-core processes, respectively.

Fig. 2 suggests the need to investigate more in hard-core and soft-hard-core nucleation processes in formal kinetics theory. A first step in this direction is to consider and compare transformed regions driven by nucleation processes modelled by Matérn I and Strauss hard-core processes. For sake of simplicity, let us consider a site-saturated nucleation process with spherical exclusion zone

with radius R, and ellipsoidal growth model as defined in Section 2.2. The causal cone $\mathcal{C}(t,x)$ of a point x at time t is then given by

$$\begin{aligned}\mathcal{C}(t,x) &= \{(y,\phi) \in \mathbb{R}^3 \times SO(3) \,:\, x \in \Theta_0^t(y,\phi)\} \\ &= \{(y,\phi) \in \mathbb{R}^3 \times SO(3) \,:\, y \in x + Gt\mathcal{E}_0(a,\phi)\}\end{aligned}$$

Let $N = \{(x_i,\phi_i)\}$ be a site-saturated nucleation Poisson point process in $\mathbb{R}^3$ with marks in $SO(3)$, modelling centres and orientations of the ellipsoidal grains, with intensity measure $\Lambda(\mathrm{d}(x,\phi)) = f(x)\mathrm{d}xQ(\mathrm{d}\phi)$. We denote by N_{Str} and by N_{Mat} the marked Strauss and the Matérn hard-core processes with underlying Poisson point process N, respectively. That is the unmarked point process of the locations, say $\widetilde{N}_{Str}$ and $\widetilde{N}_{Mat}$, respectively, are the Strauss and the Mateérn hard core process with minimal interpoint distance R driven by the unmarked Poisson point process $\widetilde{N} = \{x_i\}$ defined as above. Then the intensity measure of N_{Mat} will be of the type

$$\Lambda_{Mat}(\mathrm{d}(x,\phi)) = f_{Mat}(x)\mathrm{d}xQ(\mathrm{d}\phi),$$

whereas the intensity measure of N_{Str} will be of the type

$$\Lambda_{Str}(\mathrm{d}(x,\phi)) = f_{Str}(x)\mathrm{d}xQ(\mathrm{d}\phi).$$

It can be shown [18] that

- $f_{Mat}(x) = f(x)e^{-\Lambda(B_R(x))}$.
  (As a consequence, if f is of the type (10), then $f_{Mat}(x) = f(x)e^{-\frac{4}{3}\pi R^3 f(x)}$.)
- $f_{Str}(x)$ is not explicitly computable because it turns out to be expressed in terms of the untractable normalizing constant α which appears in Eq. (19). Nevertheless, by specializing a more general result in [18], it holds

$$f(x)e^{-\Lambda(B_R(x))} \le f_{Str}(x) \le \frac{f(x)}{1 + \int_{B_R(x)} e^{-\Lambda(B_R(y)\cap B_r(x)^c)} f(y)\mathrm{d}y}.$$

Hence, the following relation holds between the intensities of the unmarked involved point processes:

$$f_{Mat}(x) \le f_{Str}(x) \le f(x) \qquad \forall x \in \mathbb{R}^3.$$

Let us denote by $V_{E,Mat}(t,x)$, $V_{E,Str}(t,x)$ and by $V_E(t,x)$ the mean extended volume density at x at time t of the transformed region associated to the nucleation process N_{Mat}, N_{Str} and N, respectively. Hence, by remembering (9), we conclude

$$\begin{aligned}V_{E,Mat}(t,x) = \Lambda_{Mat}(\mathcal{C}(t,x) &= \int_{SO(3)} \int_{x+Gt\mathcal{E}_0(a,\phi)} f_{Mat}(y)\mathrm{d}yQ(\mathrm{d}\phi) \\ \le V_{E,Str}(t,x) = \Lambda_{Str}(\mathcal{C}(t,x) &= \int_{SO(3)} \int_{x+Gt\mathcal{E}_0(a,\phi)} f_{Str}(y)\mathrm{d}yQ(\mathrm{d}\phi) \\ \le V_E(t,x) = \Lambda(\mathcal{C}(t,x) &= \int_{SO(3)} \int_{x+Gt\mathcal{E}_0(a,\phi)} f(y)\mathrm{d}yQ(\mathrm{d}\phi).\end{aligned}$$

We recall that the void probabilities of a point process Φ in $\mathbb{R}^d$ are the probabilities of the type $\mathbb{P}(\Phi(A) = 0)$ for any compact $A \subset \mathcal{B}_{\mathbb{R}^d}$. Unfortunately, for the time being, explicit expressions for the void probabilities of Strauss and Matérn hard-corse processes are not available in the literature. As a consequence we do not have a relation between $V_{V,Str}(t,x)(= 1 - \mathbb{P}(N_{Str}(\mathcal{C}(t,x)) = 0))$ and $V_{V,Mat}(t,x)$. Of course both $V_{V,Mat}(t,x)$ and $V_{V,Mat}(t,x)$ are less than $V_V(t,x)$ for any $(t,x) \in \mathbb{R}_+ \times \mathbb{R}^3$; by simulation studies in [18] we have $V_{V,Mat}(t,x) \leq V_{V,Str}(t,x)$, as intuitively one expects by the same relation for the mean extended volume densities.

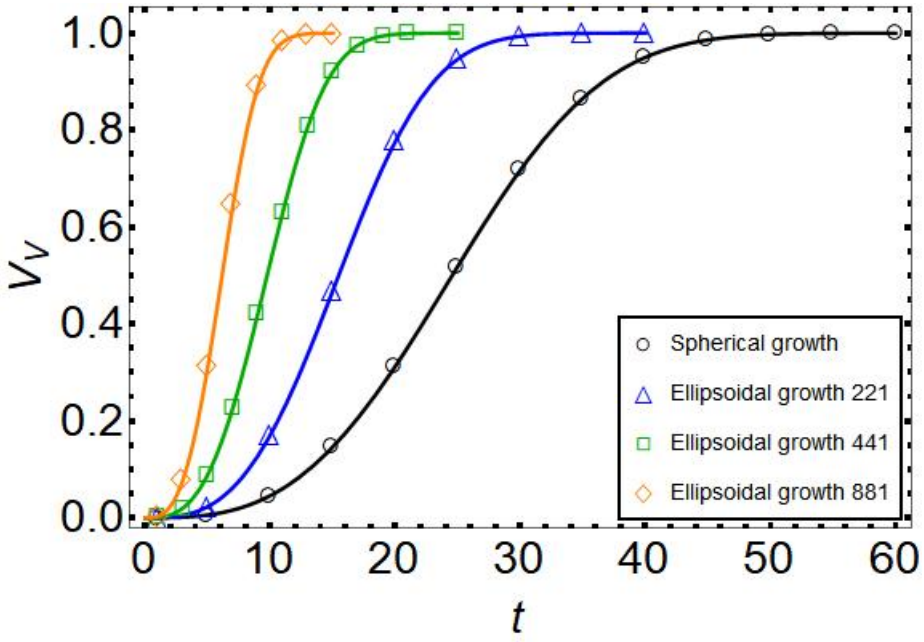

Fig. 1. Comparison of the mean volume density against time (in dimensionless units) between ellipsoidal growth with four different aspect ratios. Spherical growth means a ball growing with: $a_1 = 1, a_2 = 1, a_3 = 1$. The other ellipsoids are oblate ellipsoids in which the larger axes and smaller axes are: $a_1 = 2, a_2 = 2, a_3 = 1$, $a_1 = 4, a_2 = 4, a_3 = 1$, and $a_1 = 8, a_2 = 8, a_3 = 1$. In all cases, the nucleation took place at points located in space according to a homogeneous Poisson point process.

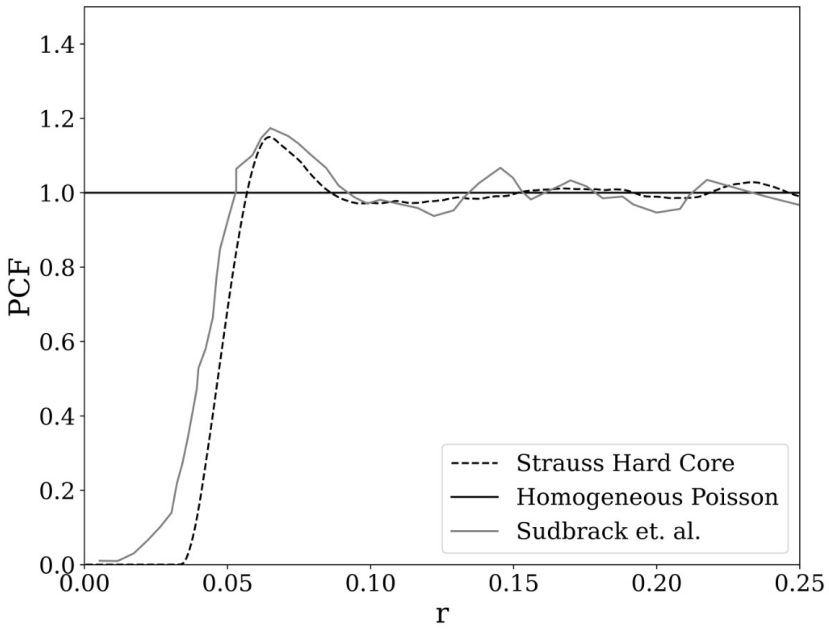

Fig. 2. Comparison of the pair correlation function of the experimental work of Sudbrack *et al.* [23] with that one of a simulated Strauss hard-core process.

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