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Criticality of trapping in a dynamic epidemic model

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Abstract. We study a simple model mimicking the two-dimensional growth of a solid interface B through a liquid L in presence of particles A which are pushed by the advancing front. The model considers a short-range repulsive interaction between the particles and the advancing front (the so-called Uhlmann, Chalmers and Jackson mechanism). As particles are pushed by the advancing front, this leads to the formation of aggregates which are hindrances to the growth and which can be trapped leading to the formation of internal patterns. A transition between indefinitely growing clusters and frozen ones takes place for a critical particle fraction $x_c = 0.560 \pm 0.005$ which is larger than the critical fraction of the corresponding epidemic model with static particles. At that critical threshold x_c, both percolating clusters and internal patterns are numerically found to be fractal with the same dimension $D_f = 1.87 \pm 0.03$ close to the classical percolation exponent 91/48. The correlation length exponent ν is found to be $\nu = 1.34 \pm 0.08$ close to the classical percolation exponent 4/3. The criticality of the internal patterns is unexpected.

Aggregration of particles is a common phenomenon in nature [1]. During the past decades, much work has been done in order to understand the kinetics and growth morphologies of various aggregates. Several models such as the diffusion-limited aggregation (DLA) [2] and the cluster–cluster aggregation (CCA) models [3] have been imagined. The structures of the aggregates have been well described through the fractal [4] and multifractal concepts [5].

However, less attention has been paid to the aggregation of particles pushed by an advancing interface due to some repulsion. The repulsive short-range interaction between a solidifying front and a single particle has previously been studied by Uhlmann, Chalmers and Jackson (UCJ) [6]. The UCJ mechanism was intended to describe the trapping or not of a single particle depending on the particle size, the interfacial free energies and the growth rate of the interface [6]. For a given value of the growth rate and of the interfacial liquid/particle, liquid/solid and particle/solid free energies, it was found that there exists a critical particle size below which a particle can be indefinitely pushed by the front and above which a particle is trapped in the crystal matrix. However, the physics of the multiparticle problem with possible aggregation was never considered to our knowledge.

Such a multiparticle problem is of great interest in, for example, the field of crystal growth and, more precisely, for the decoration of a crystal with impurities or secondary phases [7]. The basic example of this is the growth of a crystal from a melt [8], i.e. the growth of a solidifying phase B from a liquid phase L following the basic reaction

$$L \rightarrow B \tag{1}$$

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taking place in the presence of impurities (or particles) of solid phase A. This is the case of, for example, organic crystal growth in the presence of metallic particles [6]. The case of carbon nanotube growth in the presence of cobalt particles could also be related to this work [9]. One should note that up to now in the literature, most examined reactions look as 'theoretically simple' as equation (1) [10]. Another but more complex case is that where the A-particles are partially or not consumed in the chemical reaction

$$A + L \rightarrow B \tag{2}$$

which is that of an incomplete or not peritectic reaction. Sometimes unconsumed A-particles are trapped by the advancing front. Such an incomplete peritectic reaction is, for example, encountered in superconducting $YBa_2Cu_3O_{7-\delta}(\equiv B)$ compounds [11, 12]. The A-particles (made of the non-superconducting phase Y_2BaCuO_5) are known to influence electrical properties such as the critical current density J_c [13]. Thus, the incomplete reaction (2) is of interest.

It is therefore of interest to examine case (2) in which particles can furthermore be pushed away leading to an aggregation process on the front. In such a case, the characteristics of the aggregates of particles trapped by the front should be studied. A simplification used here will be to consider the A-particles to be chemically inactive and of constant size. We thus propose a growth model which considers a UCJ-like mechanism, i.e. a repulsive short-range dynamical interaction between a growing front and particles. To our knowledge, this is the first time that a UCJ-like process has been implemented in a growth model for a multiparticle system. The model is constrained to be as simple as possible. The number of A-particles is fixed to be a constant. This inactivity is valid to model equation (2) if the A-particles are large enough to be not totally consumed by the reaction (2), i.e. if the dissolution rate of the A-particles is slower than the growth rate of the B-phase (as in the melt-texturation process of $YBa_2Cu_3O_{7-\delta}$ compounds). This restriction, however, allows for various extensions and applications in further work. Beside the time dependence of the A-particle concentration and extensions to other types of interfaces (such as two unmixing fluids) are obvious, non-solid particles can also be envisaged such as non-coagulating liquid droplets or vesicles. Many other spreading phenomena (epidemia, dielectric breakdown, gelation, etc) are covered by the present study. In the following, we will discuss the model in terms of a solid/liquid interface because it is more traditional for the UCJ mechanism.

The model was specifically studied on a square lattice ($d = 2$) where each site can receive a liquid unit (phase L), a solid unit (phase B) or a particle (phase A). One should note that in the present model, one site can contain at most one phase or one particle. Initially, all sites are turned into the liquid phase except for a fraction x of sites which each contain an A-particle. The initial spatial distribution of particles is supposed to be random. The growth is initiated by flipping one liquid unit into the solid state (B) at the centre of the lattice (following the reaction of equation (1)). At each simulation step, all liquid sites in contact with the so-called cluster (B) are selected. One of them is randomly chosen and is turned into the solid state of phase B (following equation (1)). Such a mechanism is equivalent to a classical Eden growth [14]. The UCJ-like mechanism is then introduced as follows. If a particle is touched by the newly added solid unit, the former makes a random move towards a nearest-neighbour liquid site reducing the contact with the solid front. This is relevant if we consider that all particles are smaller in size than the UCJ critical particle. If the particle cannot reduce its number of nearest-neighbouring solid units by such a jump, the position of the particle remains unchanged and is trapped by the front in the cluster.

One should note that a particle can be trapped in two different ways: (i) a particle can be trapped directly by the front because the former one cannot reduce its number of

nearest-neighbour solid units; or (ii) the displacement of a particle can be forbidden by the presence of other particles on neighbouring sites leading further to the trapping. This is physically relevant for a particle size smaller but close to the UCJ critical size since the pushing of aggregates is not considered here.

The selection, growth and particle motion process described here above is then repeated a desired number N of times if possible. Indeed, the growth can sometimes stop if there is no liquid site in contact with the cluster. The growth is irreversible (i.e. far from equilibrium) and history dependent (i.e. non-Markovian).

Before numerically investigating the model, let us emphasize the expected cases for particular parameter values. Without particles ($x = 0$), the model trivially reduces to the most simple version of the Eden model [15]. In such a case, a round and compact cluster grows indefinitely and fills the entire available space on the lattice. Another particular case arises when the UCJ mechanism is neglected, all particles are then static and the model reduces to the simple epidemic model [16]. We recall that for the epidemic (e) model, a transition of the random percolation universality class takes place at the critical fraction $x_c^{(e)} \simeq 0.407$ above which the cluster cannot grow indefinitely and below which the cluster (or epidemia) can grow for ever. At this critical fraction $x_c^{(e)}$ of the static particles, the growing clusters (or epidemia) are fractal with a fractal dimension $D_f = 91/48$ [16] corresponding to the fractal dimension of unconstrained percolation [17]. Thus, the difference between the epidemic and the present model is that the latter one allows for a spatial reorganization of the particles. One expects to observe in the present model the formation of particular structures of particles.

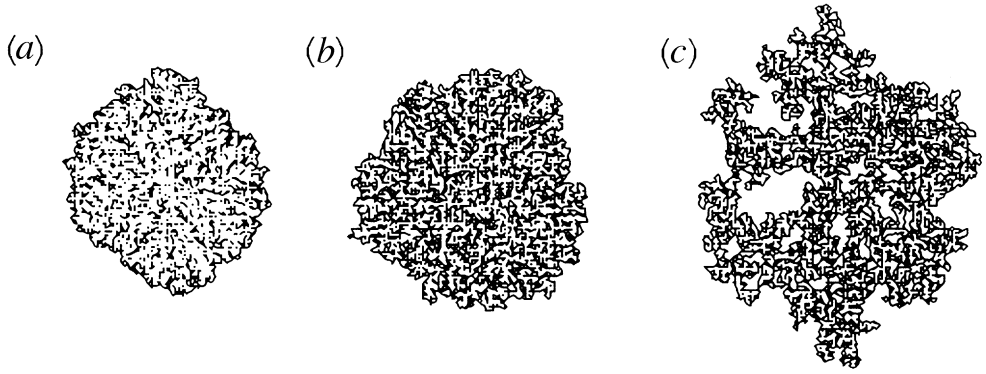

Figure 1. Three clusters of size $N = 10\,000$. The external perimeter as well as the trapped particles are drawn. Three different values of the parameter x for the initial (random) distribution of A particles are illustrated: (a) for $x = 0.20$; (b) for $x = 0.41$ which is close to the critical value $x_c^{(e)}$ of the epidemic model; and (c) for $x = 0.56$ close to the critical value of the present model.

Figure 1(a)–(c) presents three typical clusters containing each $N = 10\,000$ solid B units (white spots) for three different values of the parameter x. The perimeter of the cluster and the trapped particles are drawn in black. For a low but not negligible particle fraction, the aggregation of A-particles is clear and leads to filamentary patterns with a radial symmetry (see figure 1(a)). The shape of the growing B clusters is round as in the Eden clusters. For $x = 0.41$, i.e. just above the threshold $x_c^{(e)}$ of the static epidemic model, the cluster is still found to grow for ever. A cluster growing at this concentration is drawn in figure 1(b). Moreover, internal substructures are more tortuous. The surface is still round. When the

fraction x of particles increases above $x = 0.41$, one observes that the front becomes more jagged (as seen in figure 1(c) for $x = 0.56$) indicating that the cluster has larger hindrances to bypass. Some liquid regions of the lattice have not been reached by the growing front but are surrounded by the B solid phase. It is of interest to know whether the growth stops above some finite value $x_c > x_c^{(e)}$.

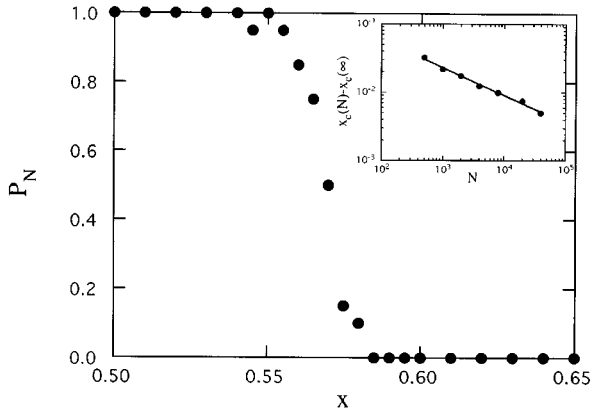

Figure 2. The probability P_N of finding a B cluster of size N as a function of the fraction x of particles for clusters of size $N = 20\,000$. Each dot was estimated by simulating 40 clusters. The inset presents the estimated critical value $x_c(N)$ as a function of the cluster size N. The continuous curve is a power law slowing down of $x_c(N)$ towards the asymptotic value $x_c(\infty) = 0.56$.

In order to estimate whether such a threshold exists, we have investigated the probability $P_N(x)$ that a B-cluster can reach a finite size N. Figure 2 shows the x-dependence of this probability estimated with clusters of size $N = 20\,000$. A well marked transition occurs at some $x_c(N)$ value close to 0.56 which is much larger than the epidemic threshold. The transition looks a little bit sharper for higher N values (not shown) but we can consider that the error bars are already short enough with such an $N = 20\,000$ illustrated size.

We interpret the high value of $x_c(> x_c^{(e)})$ as a result of the aggregation phenomenon occurring on the cluster surface. Indeed, the displacement of the particles along the front and their aggregation leaves behind some voids. The distribution of trapped particles is not uniform behind or along the front. Although the front is slowed down by the aggregates of particles, the growing front can still be locally free of particles in between the aggregates. The aggregation of particles and the growth are thus still both possible at $x = x_c^{(e)} \approx 0.41$ as clearly seen in figure 1(b). However, as the fraction x of particles increases, the displacement of the particles becomes strongly limited by the presence of neighbouring particles. Therefore, for $x > x_c$, the accumulation of particles pushed by the interface is more homogeneous along the front. The latter becomes blocked after some steps and the growth stops. The 'transition' occurring at $x = x_c$ is understood to be the result of the impossibility of easily moving a particle more than one lattice unit away from its original location. Therefore, this creates a blocking front. This is in contrast to the epidemic model in which the origin of the transition is due to the impossibility of finding an infinite path through a random pattern of static particles. Thus, the physical origins of the transition in the epidemic and the present model are 'slightly' different.

The size dependence of $x_c(N)$ was examined for $10^2 \leqslant N \leqslant 10^5$. The N-dependence is drawn in the inset of figure 2. It seems that $x_c(N)$ behaves like a power law and slows

towards an asymptotic value $x_c(\infty) = 0.560 \pm 0.005$. This power law slowing down is emphasized in the inset of figure 2 and holds over two decades. The exponent of this slowing down behaviour was estimated to be 0.40 ± 0.03.

Finite-size scaling arguments of classical percolation [17] equate the connectivity length $\xi \sim (x_c - x)^{-\nu}$ with the cluster characteristic size N^{1/D_f} resulting in the relation

$$x_c(\infty) - x_c(N) \sim N^{-1/\nu D_f} \sim N^{-0.4} \tag{3}$$

This gives a direct measure of the product νD_f. For $x < x_c(\infty)$, the clusters of B units are found to be compact and filling the available space such that the fractal dimension of these is trivially $D_f = d = 2$.

In order to find D_f and ν, we have investigated how the resulting structure scales at criticality (for $x = x_c(\infty)$). Radial density functions $\rho_A(r)$ and $\rho_B(r)$ have been calculated. They represent the probability of finding at a distance r from the centre of the lattice a trapped particle A or a B unit respectively. We recall that the centre of the lattice is the position of the initial growth site turned into phase B. Figure 3 presents the radial density functions $\rho_A(r)$ and $\rho_B(r)$ in a log–log plot averaged over 20 clusters of $N = 80\,000$ units grown with a fraction $x = 0.56 \approx x_c(\infty)$. Because of the finite size of our clusters, the radial density functions present a marked cut-off around $r = 250$. The density functions are found for $5 < r < 250$ to be power laws for both the cluster sites B and the trapped A-particles.

$$\begin{aligned} \rho_A(r) &\sim r^{-\alpha} \\ \rho_B(r) &\sim r^{-\beta} \end{aligned} \tag{4}$$

where the exponents are numerically found to be the same ($\alpha = \beta$) over two decades. For $x = x_c(\infty)$, the ratio ρ_A/ρ_B is found to be a constant and equal to about $\rho_A/\rho_B = 0.89$.

A power law for the density function indicates that an aggregate is fractal with a dimension $D_f = d - \alpha$ [18]. The fractal dimension of both the solid A and B phases are found to be numerically the same, i.e. $D_f = 1.87 \pm 0.03$ which is close to $91/48 \approx 1.896$ within error bars. With this value for D_f, the critical exponent ν is found to be $\nu = 1.34 \pm 0.08$ (see equation (3)), a value which is close within error bars to the unconstrained percolation exponent $\nu = 4/3$ [17].

One should note that for very small r values, all sites contain a solid phase A or B (whence no liquid) such that the relation $\rho_A(r) + \rho_B(r) = 1$ is verified. The fractal growth only occurs for $r > 5$ (see figure 3). Indeed, the first A-particles are easily pushed in the earlier stages of the growth forming the first aggregates of phase A at a distance $r > 0$. This explains why $\rho_A(r)$ is very small for small r values (see figure 3).

We have also investigated the evolution of the number t_A of trapped A-particles (particles which are in contact with the B-cluster and which cannot move) as a function of the cluster size N (see figure 4). For $x \leqslant x_c(\infty)$, the evolution of $t_A(N)$ in the growing cluster is numerically found to obey the empirical relation

$$t_A = cN - c'N^{\gamma} \tag{5}$$

where c and c' are two parameters which are functions of x only. The first term expresses an increase in the number of trapped A-particles proportional to the size N of the bulk B-cluster. The second term represents the aggregates of A-particles lying on the surface of the growing cluster, particles which are blocking the front.

The sites in contact with the B-cluster are either L sites which are candidates for the growth or contain an A-particle. For $x < x_c(\infty)$, both the number of site candidates for the growth and the number of A-particles on the surface increase with N and behave like

the perimeter size which is proportional to $N^{1/2}$ since $D_f = 2$. For $x = x_c(\infty)$, the growth is critical and the total number of sites which are candidates for the growth is expected to be roughly independent of N. In this case, the number of A-particles lying on the surface of a B-cluster is a power of N with an exponent expected to be $(D_f - 1)/D_f$ [18]. If the number of trapped particles on the surface is proportional to the total number of A-particles lying on the surface, this leads to an exponent

$$\gamma = (D_f - 1)/D_f \tag{6}$$

expected to be exactly 1/2 for x below $x_c(\infty)$ and $43/91 \approx 0.472$ for $x = x_c(\infty)$.

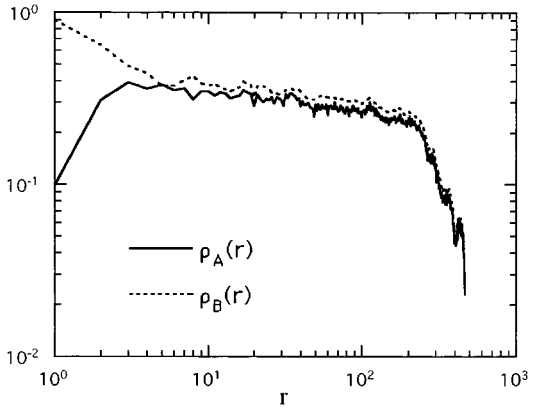

Figure 3. Log–log plot of the density functions $\rho_A(r)$ and $\rho_B(r)$ for respectively the cluster sites B and the trapped A-particles at the critical fraction $x_c(\infty)$. Each dot is an average over 20 simulated B clusters of size $N = 80\,000$.

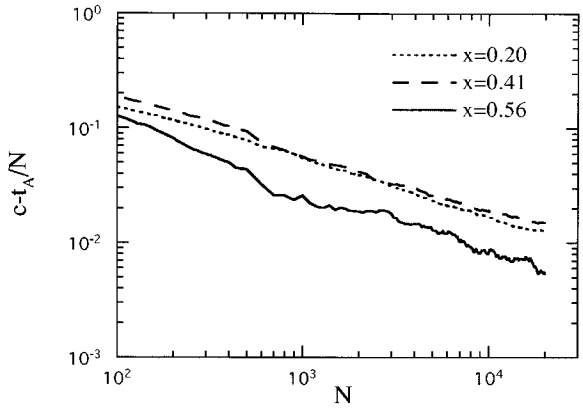

Figure 4. Log–log plot of the evaluation of $(c - t_A/N)$, i.e. a function of trapped particle concentration t_A/N as a function of N for respectively $x = 0.20$, $x = 0.41$ and $x = 0.56$. Each curve is an average over 40 simulated clusters.

Figure 4 presents a log–log plot of the evolution of $(c - t_A/N)$ as a function of N for $x = 0.20$, $x = 0.41$ and $x = 0.56 \approx x_c(\infty)$ respectively. Each curve results from an average of over 40 clusters. Power laws are well observed and hold over more than two decades. The exponent $\gamma - 1$ can be deduced. Table 1 summarizes the results of the fit

of these three curves by the relation of equation (5). The agreement between the fitted γ values and the expected values (1/2 and 43/91) from equation (6) is remarkable.

Table 1. The values of the parameters in equation (5) fitting the curves of figure 4.

x	γ	c	c'
0.20	0.505 ± 0.015	0.25 ± 0.01	1.68 ± 0.05
0.41	0.501 ± 0.015	0.60 ± 0.01	1.95 ± 0.05
0.56	0.465 ± 0.020	0.89 ± 0.01	1.53 ± 0.08

In conclusion, we have introduced here an original mere two-dimensional model of growing interfaces considering a short-range repulsive (UCJ-like) interaction between the growing front and some chemically inactive particles. The model allows for many extensions and applications in the epidemic, catalysis [9] and fluid spreading phenomena fields. For example, the dissolution of particles will be considered in a further work. The growing interface pushing the particles leads to a non-trivial aggregation phenomenon and to the formation of non-trivial patterns made of trapped aggregates.

A transition between unlimited and limited growing clusters takes place at some particle fraction $x_c(\infty)$ which is larger than the static percolation value $x_c^{(e)}$ of the epidemic model. We have emphasized the different origins for the transition in the present and in the classical epidemic model. For the epidemic model, the origin of the transition is the impossibility for $x > x_c^{(e)}$ to find an infinite path through a random pattern of particles. For the present model, the origin of the transition is the possibility for the particles to aggregate sufficiently for $x < x_c$ in order to leave free regions for cluster growth. For x approaching $x_c(\infty)$, the aggregation phenomenon is, however, found numerically to be driven by the critical exponents of static percolation. The process is critical for both cluster growth and aggregation phenomena and results in the fractality of the internal patterns made of trapped particles. The fractal dimension of the pattern is found to be identical to that of the cluster. The criticality (or the fractality) of the aggregation phenomenon was unexpected. This critical patterning belongs to the universality class of two-dimensional unconstrained percolation.

Beside these numerical results, we have seen the emergence of complex patterns from rules not especially introduced for that purpose. Indeed the rules of the present model consider only the growth and an UCJ-like mechanism. We recall that the action of local physical rules on multiparticle (or species) systems can sometimes lead to collective behaviours [19] as observed here. The latter processes can develop structures that appear to have order on all length scales. Such resulting patterns and dynamic processes seem to be common events in nature and in living systems. The present model could be replaced in the general context of studying natural pattern formation.

Acknowledgments

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