Surface properties and scaling behavior of a generalized deposition model

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The surface exponents, the scaling behavior and the bulk porosity of a generalized ballistic deposition model of physically realistic particles is studied. Particles in nature have varying degrees of stickiness ranging from completely non-sticky to fully sticky. A model of deposition of such realistic particles should allow for non-sticky random-like, strongly sticky ballistic-like and all other interim possibilities. Such a generalized model forms a super set of the competitive growth models studied in the literature and incorporates several new configurations. In this article we find the scaling exponents for surface width and porosity. In terms of scaled width \( \ln W \) and scaled time \( \ln t \) the numerical data collapse on a single curve for widely varying sticking parameter \( p \) and system size \( L \). Similar scaling is also found for the porosity.

I. INTRODUCTION

The formation and growth of rough surfaces have several applications in physical and chemical processes, such as, crystal growth, growth of thin films, vapor deposition, formations of colloids and electroplating to name a few [1, 2]. Many of the unique mechanical, optical and electromagnetic properties of surfaces originate from their surface morphology. The bulk properties of depository rocks, e.g., porosity, saline saturation, texture, stability and strength find important applications in geology of sedimentary rocks. The underlying formation mechanism influences the geometry of deposition structures and is relevant in the manufacture of optical and electronic nanostructures and nanodevices, sophisticated drug delivery systems using magnetic carbon nanostructures [3] and smart nanostructures for monitoring, diagnoses and treatment in physiology [3]. Understanding the dynamics and growth of surfaces is, therefore, a challenging problem in surface science.

There are two fundamental approaches to the study of surface growth: (i) extensive numerical simulation of discrete models and computation of surface and bulk properties [2]; and (ii) solving the stochastic differential equation derived from phenomenology corresponding to the growth model [1, 6]. Another recent approach of study involves transformation of discrete deposition rules into stochastic differential equations using a limiting procedure and regularization, and hence finding the scaling exponents [7].

Random deposition (RD) is a simple deposition process where non-sticky, solid particles deposit on randomly selected sites of a substrate. A quantitative measure of the roughness of the surface, called the surface width \( W(L, t) \), is defined in terms of the surface height \( h(i, t) \), at a site \( i \) and at a time \( t \), as,

\[
W(L, t) = \sqrt{\frac{1}{L} \sum_{i=1}^{L} (h(i, t) - \langle h(t) \rangle)^2}, \tag{1}
\]

where \( L \) is the system size, and \( \langle \cdot \rangle \) is the average. In RD, each site grows independently of the other sites and the surface roughness grows without bound. There are no voids in random deposition, so the deposition structure is compact [1].

Ballistic deposition (BD) on the other hand, gives rise to porous structures as the depositing particles stick to the first surface they encounter in their vertical downward journey towards randomly selected sites. In BD, the particles behave as strongly sticky, whereas in RD they are not sticky at all [1, 8, 9]. In nature however, particles may have intermediate stickiness which varies between the two extremes of strongly sticky and completely non-sticky behavior.

In this work, we present a generalized ballistic deposition model (GBD) to study the deposition of particles with physically realistic intermediate stickiness. The varying degrees of stickiness of the particles is introduced by means of a parameter \( p \) with values ranging from 0 to 1; the former representing non-sticky and the latter representing extreme stickiness. Here, a particle is dropped vertically towards a randomly selected site on the substrate. The particle sticks to the first surface of contact it encounters with a probability \( p \) or continues its downward journey with a probability \( 1 - p \). The descending particle then sticks to the very next site of contact with probability \( p(1 - p) \), or continues to the next lower position with probability \( (1 - p)(1 - p) \). This process continues till the particle either sticks to a site of contact or it reaches the bottom of the column. This deposition mechanism is illustrated in Fig 1f. The arrow indicates the selected site. The grey boxes numbered 1, 2, 3 . . . are the possible positions where a new particle may stick with probabilities \( p, p(1 - p), p(1 - p)^2 \cdot \cdot \cdot \) respectively. For

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sticking probability $p = 0$, its minimum value, the GBD corresponds to RD (Fig 1a), while at the highest value, $p = 1$, it corresponds to BD (Fig 1b). A logarithmic plot of the surface width $W(L, t)$ versus $t$, for GBD shows four distinct regions; an initial random growth, an intermediate rapid growth growing faster than random [12, 13], followed by a KPZ-like growth [6] and a subsequent saturation.

The initial random growth is independent of both the sticking probability $p$ and the system size $L$. The intermediate region of rapid growth, that starts in the later stages of sub-monolayer growth and continues till a few layers of particle deposition, is dependent on the probability of sticking. With further deposition, the steep increase of roughness slows down to KPZ-like growth and eventually saturates. The saturation region and the KPZ-like growth region preceding it, depend strongly on the sticking probability and the system size. An interesting scaling relation of surface roughness with both the system size $L$, and the sticking probability $p$, is found in these two regions as,

$$W(L, p, t) \sim L^\alpha p^{-\alpha' G(t/\gamma L^z)},$$

where $F(x)$ is a scaling function that satisfies $F(\infty) \sim constant$ and $F(x) \sim x^d$ for small $x$. As in BD, the present model, for any $p > 0$, leads to porous structures [14]. Hence, a porosity $\rho$ may be defined as the fraction of unoccupied sites within a certain number of layers, just below the active interface, where no further deposition can take place. The porosity $\rho$ is studied both in the growth and saturation regions. It increases with increase in $p$ and shows a very weak dependence on $L$. A scaling relation is found for the porosity, that combines its dependence on both the sticking probability $p$ and system size $L$ as,

$$\rho(L, p, t) \sim L^a p^b G(t/\gamma L^z).$$

$G(y)$ is a scaling function that satisfies $G(\infty) \sim constant$ and $G(y) \sim y^d$ for small $x$.

The GBD studied in this work is distinct from the competitive growth models in literature [10, 11, 15–23]. Competition between growth models is introduced by considering different species of particles or by one type of particle following different growth mechanisms. In the competitive growth models involving one type of particle, a competition between two growth mechanisms, such as RD and BD is introduced. The incoming particle deposits on first contact as in BD, with some chosen probability, or simply deposits on top of selected site as in RD. Thus, the possible positions of the new deposit are far fewer when compared to GBD studied in this present work. Our present model includes not only the configurations appearing in the competitive growth models, but also allows several other physically admissible ones. Thus, the configurations possible in the competitive growth models (Fig 1c, 1d, 1e) simply form a small subset of the large ensemble of configurations allowed in the present model (Fig 1f).

In our simulations of the present generalized deposition model, two independent random number generators were used, one for selecting a site on the growing surface and, another to determine whether a particle will stick at a particular location for a chosen value of the sticking probability. These two random number generators are completely independent and uncorrelated to each other.

II. GENERALIZED BALLISTIC DEPOSITION MODEL

The generalized ballistic deposition model presented in this work attempts to represent the deposition of realistic particles with varying degrees of stickiness. A parameter $p$, whose values vary between 0 and 1, is introduced in
the GBD, that represents the probability of an incoming particle sticking to a point of contact on the growing surface. In this model, a particle is allowed to descend vertically towards a randomly chosen site on a one-dimensional substrate. If the selected site is higher than its nearest neighbors, the particle simply deposits on top of the column at that site. However, if the chosen site has a taller column of particles as its nearest neighbor, then the new particle sticks to the first occupied site it encounters if the value of $p$ is larger than a random number generated from a uniform distribution between 0 and 1. Otherwise, it slides down vertically to the next occupied site with probability $(1-p)$. At this site the particle may stick with probability $p(1-p)$ or continue its further descent with probability $(1-p)^2$, and so on, till it reaches the bottom. Thus if the chosen site has a nearest neighbor with column height taller by $n$ layers relative to it, the probabilities of the arriving particle sticking to the successive particles of the nearest neighbor column from top are given by,

$$P(1) = p, \quad P(2) = p(1-p), \ldots \quad P(k) = p(1-p)^{(k-1)}. \quad (4)$$

The probability that the particle slides past the preceding $(n-1)$ occupied neighbors, and lands at the lowest possible position is given by,

$$P(n) = 1 - \sum_{k=1}^{n-1} P(k) = (1-p)^{(n-1)}.$$

This describes a proper stochastic process. The total probability of a descending particle sticking to one of the allowed position is $\sum_{k=1}^{n} P(k) = 1$.

In simple deposition models, the surface width follows a dynamic scaling law [24],

$$W(L,t) \sim L^\alpha f(t/L^z), \quad (5)$$

where $f$ is a scaling function satisfying $f(\infty) \sim constant$ and $f(x) \sim x^\beta$ for small $x$. The exponents $\alpha$, $\beta$ and $z$ are related by $z = \alpha/\beta$.

For the GBD studied in this work, the introduction of a sticking probability $p$, brings in another parameter in the problem. GBD interpolates between RD ($p = 0$) and BD ($p = 1$) systems. Physically relevant quantities, e.g., surface width $W(L,p,t)$ and porosity $\rho(L,p,t)$ thus depend on the sticking probability $p$ in addition to $L$ and $t$. From the results of our simulation we obtain dynamic scaling relations,

$$W(L,p,t) \sim L^\alpha p^{-\alpha'} F\left(\frac{tp^{z'}}{L^z}\right)$$

$$\rho(L,p,t) \sim L^\alpha p^\beta G\left(\frac{tp^{z'}}{L^z}\right),$$

where $F(x)$ and $G(y)$ are scaling functions described in the previous section.

III. RESULTS AND DISCUSSION

For different values of sticking probabilities between $p = 0$ and $p = 1$, simulations were performed in $(1+1)$ dimension for system sizes $L = 32, 64, 128, 256, 512$. The average number of layers deposited is used as a measure of time $t$. The logarithmic plot of surface width with time has four distinct regions, for any non-zero probability ($p > 0$). This is shown in Fig [2].

The dependence of surface width $W$ on $t$ in log-log scale, in the early submonolayer region ($t \ll 1$) is linear with slope $1/2$ as in random deposition (growth region 1, GR-1). At later stages of submonolayer growth (growth region 2, GR-2), $t \sim 1^{-}$, the surface width shows a steep increase which continues for the first few layers $(1 - \epsilon \leq t \leq 3, 1 > \epsilon > 0)$. With deposition of further layers, the rate of increase in width slows down (growth region 3, GR-3). After deposition of a large number of layers, the ensemble average of the surface width saturates. Three different crossover times are of relevance. The first crossover time $t_c$ corresponds to the change from random growth to region with slope greater than $1/2$. The second crossover time $t_k$ corresponds to time beyond few layers where the slope decreases and changes from GR-2 to GR-3. The third crossover time $t_{sat}$ corresponds to beginning of saturation region.

The appearance of different growth regions in the present model may be understood as follows. Initially, when the deposition starts from a flat substrate almost no two adjacent sites are occupied. Hence there is no correlation among neighboring columns and the growth is random like, irrespective of whether the model allows for sticking or not. This feature is observed in all systems with different $L$ and $p$ values as shown in Fig [2] and Fig [3].

![FIG. 2: (Color Online) Logarithmic plot of surface width with time for different $p$ and system size $L = 256$, showing four distinct regions and crossover times.](image)

The deviation from random like behavior in the few layer deposition region is shown in Fig [4]. The rate of growth of surface width in this region is higher than that...
in the case of random deposition. As the number of particles deposited is nearly \( L \), due to fluctuation, some short multi-layer columns may start forming. Hence the descending particles encounter occupied neighbors, and allowing sticking in the model, brings in non-trivial correlations in the system. However, since very few layers are deposited at this stage, even one particle sticking to a higher location or descending to the bottom of a column, makes a significant relative change in width. Thus the rate of growth of surface width in this region when only a few layers have formed, is higher than that for RD. Our study shows, that the growth exponent in this region, denoted by \( \beta' \), increases with sticking probability \( p \), and is almost independent of system size \( L \), as shown in Fig 2 and Fig 3.

The rate of increase in surface width slows down as more and more particles are deposited in GR-3. The average height of the interface and its width are larger. The descending particle need not proceed to the bottom, and can get deposited at a higher location by sticking. Thus the correlation has a smoothening effect, as it fills up deep crevices efficiently. The growth exponent \( \beta \) in this region decreases with \( p \), unlike the exponent in GR-2, as seen in Fig. 5. With further deposition of particles the surface width finally saturates. The saturated width depends both on the system size \( L \) and sticking probability \( p \), as shown in Fig 2 and Fig 3.

For a given value of \( p \), the surface width at saturation \( W_{sat} \), and the time at which the saturation is reached \( t_{sat} \), increase with system size \( L \). For a given system size \( L \), \( W_{sat} \) and \( t_{sat} \) decrease with increase in probability of sticking \( p \). This decrease is more pronounced for lower values of \( p \).

The saturated values of the surface width for a given system size decrease with increase in the probability of sticking. This dependence is of the form \( W_{sat}(L,p) \sim f(L) \cdot p^{-\alpha'} \), where the exponent \( \alpha' \) is independent of \( L \) (Fig 7). An increase in sticking probability \( p \) corresponds to a stronger correlation in the deposition process. The surface width saturates at lower values of saturation width \( W_{sat} \), at corresponding earlier times, i.e., smaller \( t_{sat} \). For a given probability of sticking \( p \), \( \ln W_{sat} \) increases linearly with \( \ln L \). The dependence is found to be of the form \( W_{sat}(L,p) \sim L^\alpha \) (Fig 8). From results of extensive simulations, graphically presented in the adjacent figures, Fig 6 Fig 7 and Fig 8 we find the exponents \( \alpha = 0.452395 \) and \( \alpha' = 0.249763 \), in the region of saturated surface width.

The surface width \( W \) in the third growth region, GR-3, i.e., between \( t_k \) and \( t_{sat} \) depends on both system size \( L \) and sticking probability \( p \) as shown in Fig 9. The scaled width \( (Wp^{\beta'}/L^\alpha) \) in GR-3 shows that it is larger for larger system sizes \( (L \to 512) \) and lower probability \( (p = 0.125) \). For a given system size \( L \), \( t_{sat} \) and hence the growth region, decrease with increase in probability \( p \). The scaling of \( t \) with respect to \( p \) is obtained from Fig 9 with exponent \( z' = 0.7722 \). Log-log plot of rescaled

FIG. 3: (Color Online) Variation of \( \ln W_{sat} \) with \( \ln t \) for \( p = 0.5 \) for different system sizes.

FIG. 4: (Color Online) Deviation from random deposition behavior at later stages of submonolayer growth for \( L = 256 \).

FIG. 5: (Color Online) Dependence of \( \beta' \) and \( \beta \) on \( p \) shown for system size \( L = 512 \).
FIG. 6: (Color Online) Variation of \( \ln W_{\text{sat}} \) with \( \ln p \) plots for different system sizes \( L \).

FIG. 7: (Color Online) Variation of the saturated surface width \( \ln W_{\text{sat}} \) with \( \ln L \) for different \( p \) values.

FIG. 8: (Color Online) Scaled saturate surface width \( \ln (W_{\text{sat}}/L^\alpha) \) versus \( \ln p \). The slope is \(-0.249763\).

variables \( (WP^{\alpha'}/L^\alpha) \) versus \( (tp^{z'}/L^z) \) shows an excellent collapse of data in the growth region GR-3 and saturation region as shown in Fig 10 and Fig 11.

Analysis of our simulation data produces numerical estimates for the scaling exponents in Eq.2. The exponents are, \( \alpha = 0.452395 \), \( \alpha' = 0.249763 \), \( z = 1.45633 \) and \( z' = 3/4 \). From the scaled \( W \) versus scaled \( t \) graph in Fig 10 and Fig 11, we obtain \( \beta \approx 1.312 \) as the slope in the growth region GR-3. In Eq. 2, for small values of \( (tp^{z'}/L^z) \), we can approximate \( F(x) \approx x^\beta \), and hence

\[
W \sim L^\alpha p^{-\alpha'} \left( \frac{tp^{z'}}{L^z} \right)^\beta,
\]

giving \( \beta \) as the exponent of \( t \) in this regime. The exponents obtained above, satisfy the relations,

\[
\beta = \frac{\alpha}{z} = \frac{\alpha'}{z'}.
\]

The growth exponent \( \beta \) is approximately the rational fraction \( 1/3 \).

The porosity \( \rho \) can be defined as the fraction of unoccupied sites within a few layers \( N \) just below the active interface, where no further deposition can take place. It is seen that the porosity is quite independent when \( N \) is varied from 16 to \( L \) for a given system size \( L \). The porosity is found to initially increase with time signifying growth region and then saturates to a value \( \rho_{\text{sat}} \). The onset of saturation for porosity occurs earlier than the onset of saturation of surface width.

The porosity \( \rho \) is found to depend on the sticking probability \( p \) and shows a weak dependence on the system size \( L \). \( \rho_{\text{sat}} \) is higher for higher \( L \) at any given \( p \). However, in the early growth region, \( \rho(L,p,t) \) starts at a lower value for higher \( L \). The porosity in both the growth and saturation regions increases with increase in sticking probability \( p \); fully ballistic deposition system being
FIG. 10: (Color Online) $\ln(W p^{a'}/L^{a})$ versus $\ln(t p^{z'})$ plots for different sticking probability $p$.

FIG. 11: (Color Online) $\ln(W p^{a'}/L^{a})$ versus $\ln(t p^{z'}/L^{2})$ for $L = 512, 256, 128, 64$ and $p = 1.0, 0.7, 0.5, 0.25, 0.125$.

FIG. 12: (Color Online) $\ln\rho$ versus $\ln t$ for $L = 512, 256, 128, 64$ and $p = 1.0, 0.7, 0.5, 0.25, 0.125$.

FIG. 13: (Color Online) Scaled data shown as $\ln(\rho p^{-b}/L^{a})$ versus $\ln(t p^{d}/L^{c})$ for $L = 512, 256, 128, 64$ and $p = 1.0, 0.7, 0.5, 0.25, 0.125$.

IV. CONCLUSION

We have studied a generalized ballistic model of deposition of physically realistic particles with variable stickiness. The properties of surface width and porosity are studied in detail. We observe the presence of a non-KPZ growth region, where the dependence of the surface width on probability is different from that in the KPZ-like growth. We have obtained excellent collapse of data for the scaling of the surface width in terms of system size $L$ and sticking probability $p$ in the KPZ-like growth and saturation regions. A scaling relation and corresponding exponents are also found for the porosity, showing good collapse of scaled data.

The present model involves stochasticity at two stages. Firstly, in random selection of an active site, which corresponds to random noise applied to the site in the corresponding differential equation. The detailed mechanism of the change in height $h(x, t)$, determines the different spatial derivatives e.g., slope, curvature etc., that appear in the corresponding differential equations, such as in Kardar-Parisi-Zhang equation. In the present model an additional stochasticity is involved by assigning a second probability which determines the extent by which the height is altered. Thus the equation and the scaling behavior is expected to depend on this second probability. The sticking of an incoming particle at a site depends on the possibility that it has slipped past earlier points of contact without sticking. Thus most porous. Onset of saturation in porosity is earlier for higher sticking probability. A scaling behavior for porosity is obtained in the form of Eq.3, with the exponents $a = 0.0069, b = 0.2204, c = 0.14$ and $d = 0.59063$. The dependence of porosity on time $t$, sticking probability $p$ and system size $L$ is shown in Fig.12 and as scaled data in Fig.13.
the structure of the deposit depends on the evolution at successive stages. The continuum limit of such models may correspond to stochastic integro-differential equations \[23\], rather than to stochastic differential equations as in Edwards-Wilkinson model and Kardar-Parisi-Zhang model. Progress of further work along the above will be reported elsewhere.

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