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# Scaling behavior of the surface in ballistic deposition

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Using a dynamical scaling form for the surface fractal dimension as well as efficient algorithms for the simulation and analysis of the surface in three-dimensional ballistic deposition, we show that while the top of the surface is self-affine, the complete surface including overhangs has fractal dimension $D_f \simeq 3$. The existence of such a fractal surface is a consequence of the difficulty of closing off voids in three and higher dimensions. By studying a modified ballistic deposition model in which sticking is allowed with a given probability *p*, we show that the surface undergoes a phase transition from fractal to compact at a finite value of *p*. Our results also have implications for understanding the surface morphology in sedimentary rocks and low-temperature thin films.

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The morphology and evolution of the surface in thin-film growth has been a subject of extensive recent theoretical and experimental interest [1,2]. One particularly simple model, the ballistic deposition model [3], was originally formulated as a model of sedimentation and has also been extensively studied as a model of low-temperature thin-film growth and surface roughening [2]. In its simplest form the ballistic deposition model may be described as follows: starting with an initially flat surface, particles are sequentially dropped along randomly positioned vertical trajectories. Particles become part of the deposit at their positions of first contact.

While overhangs are known to play an important role in ballistic deposition [4], in most recent work the emphasis has been on the scaling behavior of the top of the surface *ignoring* overhangs, which is believed to be self-affine. In particular, extensive simulations of ballistic deposition on one-, two-, and three-dimensional substrates have been carried out [2] in which the scaling behavior of the top of the surface has been studied and compared with the predictions of the Kardar-Parisi-Zhang (KPZ) equation [5] as well as with other discrete growth models believed to be in the same universality class. While these results are important for understanding such ‘‘contact’’ properties as friction and wear, for other applications such as catalysis and adsorption it is important to understand the scaling behavior of the *entire* surface. However, the scaling behavior of the surface *including overhangs* has not been studied.

In this Rapid Communication, we present results for the scaling behavior of the entire surface including overhangs for ballistic deposition in three dimensions, corresponding to growth on a two-dimensional substrate. In contrast to the case of ballistic deposition on a one-dimensional substrate, for which the surface fractal dimension $D_f \simeq 1$ is the same both with and without overhangs, in three dimensions we find that the surface including overhangs is fractal with surface fractal dimension $D_f \simeq 2.9$–$3.0$. This result has important implications for our understanding of the surface and pore structure of sedimentary rocks [6–8] as well as for our understanding of the surface morphology in the growth of low-temperature thin films [9]. It also leads to a picture of the film in ballistic deposition, i.e., as a complicated set of branches and pores of all length scales up to the height of the film, which is completely different from the traditional picture corresponding to a self-affine surface. Our results also provide an explanation for the phase transition previously observed for the case of modified ballistic deposition in which relaxation is included [10].

In order to determine the scaling behavior of the surface including overhangs in three-dimensional ballistic deposition, we have carried out simulations on a cubic lattice using relatively large system sizes ($L = 2048$–$4096$) and average film heights ($\langle h \rangle \simeq 1000$). To simulate such large systems, an efficient bit-packing method was used in which each site of the cubic lattice corresponds to one bit of a 16-bit integer word. The surface sites were then determined by first identifying the nearest-neighbor connected cluster of empty sites above the surface (using a memory efficient algorithm [11] in which only two additional bits per site were required) and then identifying the surface sites as corresponding to all occupied sites that are nearest neighbors of this connected cluster.

In order to characterize the surface morphology as a function of length scale $l$ and coverage $\theta$ (where $\theta$ is the number of deposited layers, i.e., the number of deposited particles divided by the area of the substrate) we have used the box-counting method [1,12] along with the assumption of dynamic scaling [13]. For a fractal surface that is roughening during growth, one expects that the maximum length scale $\xi$ over which fractal behavior may be observed should increase with coverage as a power law, i.e., as $\xi \sim \theta^n$, where $n$ is a ‘‘coarsening’’ exponent. If $N(l,\theta)$ corresponds to the number of cubic boxes with sides of length $l$, which contain at least one occupied surface site at coverage $\theta$, then one expects $N(l,\theta) \sim l^{-D_f}$ for $l \ll \xi(\theta)$ (where $D_f$ is the surface fractal dimension) and $N(l,\theta) \sim l^{-d}$ (where $d$ is the substrate dimension) for $l \gg \xi(\theta)$. Combining these observations with the assumption of scaling [13] leads to the following dynamical scaling form for the surface box number $N(l,\theta)$,

$$N(l,\theta) = \theta^{-dn} f(l/\theta^n), \tag{1}$$

where the surface dynamic scaling function $f(u)$ satisfies $f(u) \sim u^{-d}$ for $u \gg 1$ and $f(u) \sim u^{-D_f}$ for $u \ll 1$. Equation (1)

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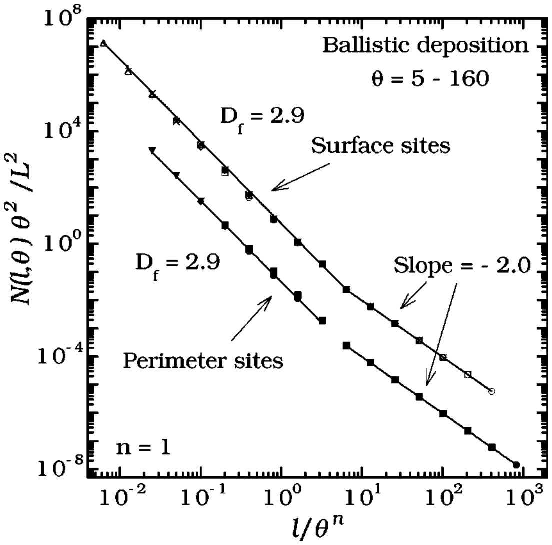


FIG. 1. Scaled surface box number as a function of scaled box size for ballistic deposition on a cubic lattice (upper symbols) along with similar results for perimeter sites (lower symbols). Perimeter site results have been shifted down by a factor of 100 for clarity.

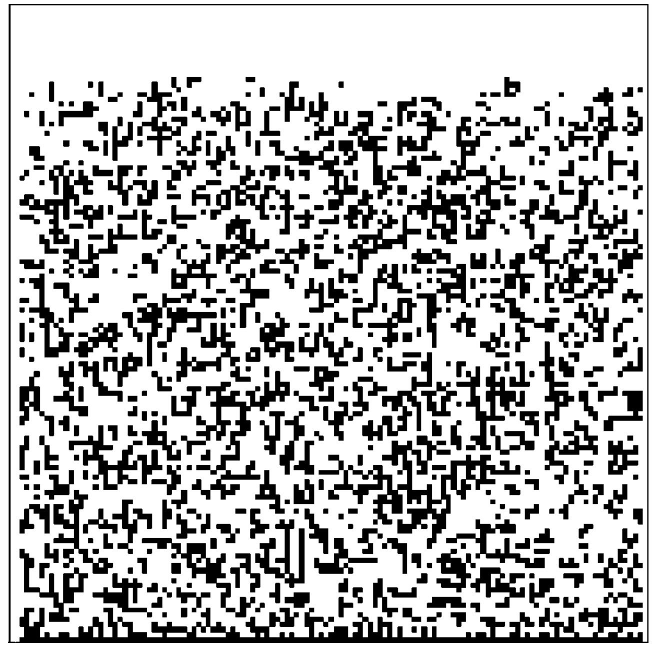

FIG. 2. Vertical cross section of ballistic deposit with system size $L=128$ and $\theta=35$.

implies that for $l \gg \xi(\theta)$, $N(l,\theta)$ is independent of coverage while for $l \ll \xi(\theta)$, $N(l,\theta) \sim \theta^{\delta}$ where $\delta = n(D_f - d)$. Assuming a small length-scale cutoff of one lattice-unit, this implies that the total surface area grows as $S(\theta) \sim N(1,\theta) \sim \theta^{\delta}$.

Figure 1 shows our results for the surface dynamic scaling function $f(u)$ for ballistic deposition on a cubic lattice ($L=2048$), over a large range of box sizes ($l=1$–$2048$) and coverages ($\theta=5$–$160$) using the value $n=1$ for the coarsening exponent. As can be seen, there is excellent scaling over almost five decades in the scaled box size and twelve decades in the scaled box number. For $l/\theta<3$, we find $D_f \simeq 2.9$ while for $l/\theta>3$ there is a sharp crossover to "flat" scaling behavior with $D_f = 2.0$. These results indicate that even though the simulated film is compact (since the average film height $\langle h \rangle$ is proportional to the coverage) the surface itself is "fractal" with fractal dimension $D_f \simeq 3$. Also shown in Fig. 1 is the dynamic scaling function for the perimeter sites corresponding to all empty sites that are nearest-neighbor sites of the surface. As can be seen the scaling behavior is essentially identical to that for the surface sites. These results contrast strongly with the corresponding results for two-dimensional ballistic deposition for which the fractal dimension $D_f \simeq 1$ at large length scales is the same whether or not overhangs are included.

In order to gain some insight into the minimum pore size, we have also measured the scaling function corresponding to the "accessible" surface sites defined as those surface sites that may be reached by traveling on the nearest-neighbor connected cluster of empty sites above the surface without touching another surface site. The accessible surface sites are thus defined in analogy to those that could be reached by an adsorbing molecule. Our results for the accessible surface sites are almost identical to those for the surface sites, thus indicating that the typical pore size is significantly larger than one lattice spacing. This is confirmed by the vertical cross section shown in Fig. 2, which illustrates the typical convoluted structure of the deposit.

How can we explain the large value of the surface fractal dimension in three-dimensional ballistic deposition? While in two dimensions, voids due to overhangs may be easily filled in due to the "joining" of nearby branches via arches, in three dimensions this is much more difficult. As a result, in three-dimensional ballistic deposition almost every deposited particle remains a part of the thin-film surface and is not blocked off. Since the film is three dimensional and compact, this implies that the surface is also three dimensional. These results lead to a picture of three-dimensional ballistic deposition, which is quite different from the standard one corresponding to a self-affine, globally flat surface. Instead, one may think of the surface of a ballistic deposit in three dimensions as a complicated set of branches and pores of all length scales up to some maximum length scale $\xi(\theta)$ that penetrates the entire film. When such branches meet or connect, they may form loops or pores but do not block off the surface.

This picture also explains the value of the coarsening exponent $n \simeq 1$. Since it is very difficult to "block" off a pore in three dimensions, the film surface extends throughout the height and width of the film. As a result, the maximum length scale corresponding to fractal behavior is only limited by the average film thickness $\langle h \rangle$, which increases linearly with coverage. For length scales smaller than the average film thickness the surface is three dimensional, while for larger length scales, the surface will appear two dimensional. In agreement with this picture the crossover from three-dimensional to two-dimensional behavior occurs at $l/\theta \simeq 3$, which corresponds (since the film density $\rho = \theta/\langle h \rangle \simeq 0.3$) to $l/\langle h \rangle \simeq 1$.

As already noted, the ballistic deposition model was originally developed as a model of sedimentation [3]. While other processes such as compaction and "antisintering" [14] play

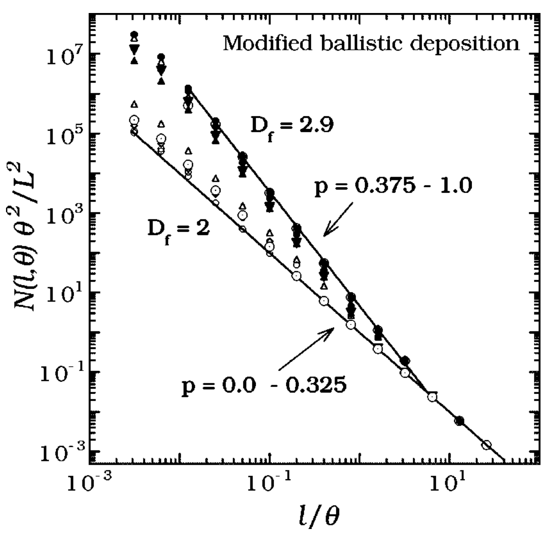


FIG. 3. Scaled surface box number as a function of scaled box size for modified ballistic deposition model ($0 \leqslant p \leqslant 1$).

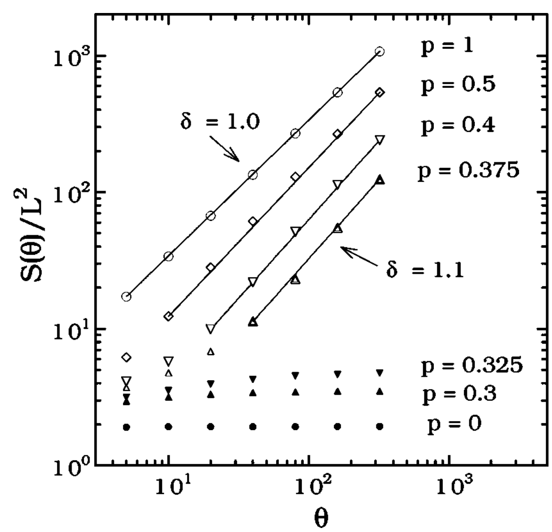


FIG. 4. Surface area as a function of coverage for different values of the sticking probability $p$ in modified ballistic deposition.

an important role in sedimentary rock formation, it is interesting that recent experimental measurements of the surface fractal dimension of sandstones [7,8] give results ($D_f \simeq 2.85$) that are relatively close to those obtained in our simple model. Similarly, measurements of the fractal dimension of the thin-film surface in room-temperature vapor deposition of gold indicate a similarly large fractal dimension $D_f \simeq 2.7$–$2.8$ [9]. Therefore, ballistic deposition may be a useful starting point to understand the development of fractal surfaces in low-temperature thin-film growth and sedimentary rocks.

In order to determine the effects of surface relaxation on the surface fractal dimension, we have also studied a modified ballistic deposition model in which each deposited particle either sticks with probability $p$ to the point of first contact, or with probability $1-p$, it falls to the lowest site within one nearest-neighbor distance of the original column. While the $p=1$ limit corresponds to pure ballistic deposition, the $p=0$ limit corresponds to Edwards-Wilkinson (EW) scaling behavior [15,16] that implies a self-affine surface with logarithmic scaling in three dimensions. The scaling behavior of the surface height fluctuations for such a model was first studied by Pellegrini and Jullien [10] who observed a transition from EW exponents for $p<0.35$ to KPZ exponents for $p>0.35$ in three dimensions. A similar transition was observed in a somewhat different model by Yan, Kessler, and Sander [17,18].

Figure 3 shows our results for the surface dynamic scaling function for the modified ballistic deposition model as a function of the sticking probability $p$. As can be seen, a phase transition from a surface with fractal dimension $D_f \simeq 3$ for large sticking probability to a flat surface with $D_f \simeq 2$ for small sticking probability is clearly indicated. In particular, for $p>0.35$ and $l/\theta<3$, the data all lie close to a line with slope $-D_f \simeq -2.9$, while for $p<0.35$ the data approach a line with slope $-D_f \simeq -2.0$. Thus, our results confirm the existence of a phase transition as a function of the sticking probability. Furthermore, they indicate that the scaling properties of the entire surface including overhangs are involved in the transition.

Figure 4 shows the corresponding results for the surface area as a function of coverage for different values of the sticking probability $p$. For $p \geqslant 0.35$, the surface area increases rapidly with $\delta \simeq 1$ as expected if every deposited particle is part of the surface, while for $p<0.35$, one has $\delta \simeq 0$. The value $\delta=1$ is consistent with the scaling relation $\delta = n(D_f - d)$ with $d=2$, $D_f=3$, and $n=1$, while in the flat phase $D_f = d$ implies $\delta \simeq 0$.

Figure 5 shows our results for the surface area growth exponent $\delta$ along with the corresponding results for the film density $\rho = \theta/\langle h \rangle$, and effective roughening exponent $\beta$ (where $w(\theta) \sim \theta^{\beta}$ and $w$ is the rms surface height) as a function of the sticking probability $p$. While all three quantities indicate the possibility of a phase transition as a function of

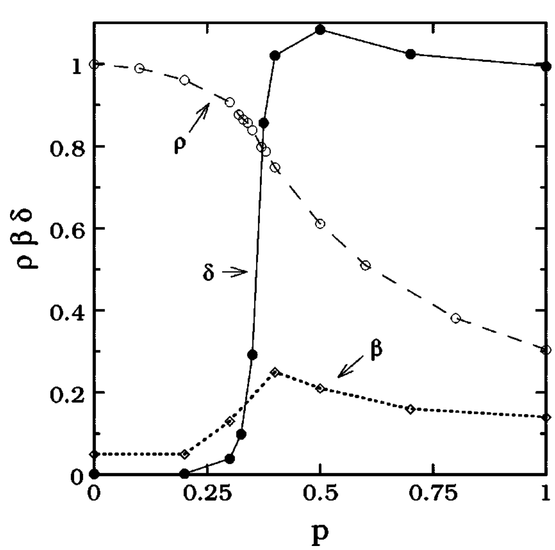


FIG. 5. Effective roughening exponent $\beta$, density $\rho$, and surface area growth exponent $\delta$ as functions of sticking probability $p$ in modified ballistic deposition.

sticking probability, the existence of such a transition is most dramatically indicated by the rapid increase in the value of $\delta$ near $p \simeq 0.35$.

Such a transition can also be interpreted as a vacancy percolation transition in $d+1$ dimensions. In this connection, we have verified that in the fractal regime, the vacancy cluster percolates in both the vertical and horizontal directions. Accordingly, one expects that at the critical sticking probability ($p_c \simeq 0.35$) the fractal dimension of the surface is the same as for three-dimensional percolation, i.e., $D_f \simeq 2.53 \pm 0.02$ [19].

In conclusion, we have investigated the scaling properties of the surface including overhangs in three-dimensional ballistic deposition. Our results show that, while the top of the surface is self-affine, the complete surface including overhangs is fractal with fractal dimension $D_f \simeq 3$. These results lead to a picture of the film in ballistic deposition, i.e., as a complicated set of branches and pores of all length scales up to the height of the film, which is completely different from the traditional picture corresponding to a self-affine surface. Due to the difficulty in blocking pores in three and higher dimensions, we expect that the same behavior should occur in higher dimensions, i.e., $D_f \simeq d+1$ for $d \geqslant 2$. Experimental results for the surface fractal dimension of sandstone and vapor-deposited gold thin films are in good agreement with our results, thus indicating that ballistic deposition may be a useful starting point to understand the development of fractal surfaces in low-temperature thin-film growth and sedimentary rocks.

We have also studied the scaling properties of the surface including overhangs for a modified ballistic deposition model. Our results explain the origin of the phase transition previously observed for this model as corresponding to an abrupt transition in the surface fractal dimension as a function of sticking probability. In the future, it would be interesting to study the effects of other relaxation mechanisms on the surface scaling behavior.

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