Roughening Transition and Percolation in Random Ballistic Deposition

Y. P. Pellegrini and R. Jullien

Laboratoire de Physique des Solides, Université Paris-Sud, Centre d'Orsay, 91405 Orsay, France

(Received 2 January 1990)

A simple ballistic model for surface growth, which considers a mixture of "sticky" and "sliding" particles, is introduced and numerically investigated in dimensions $d=2$, 3, and 4. The model exhibits, in $d=3$ and 4 (but *not* in $d=2$), a roughening phase transition, of the type recently predicted by Halpin-Healy. For the first time it is shown that such kind of surface transition is accompanied by a transition in the bulk which is characterized by a singularity in the compacity-versus-concentration curve and which occurs at the threshold of a $(d-1)$-percolation transition.

PACS numbers: 68.70.+w, 05.40.+j

Deposition of particles on surfaces is a phenomenon of considerable scientific interest with a broad range of practical applications. Even when such processes produce a compact, uniform, and nonfractal deposit, the external surface generally exhibits a rough character whose intensity varies both with lateral size of the substrate and time (proportional to the height of the deposit). The theoretical investigation of the scaling properties of surface roughness, by means of both numerical and analytical tools, is a fascinating subject which belongs to the very active field of nonequilibrium statistical physics and irreversible growth phenomena[1] where new universal behaviors are discovered.[2]

Numerical simulations of deposition processes were pioneered by Vold,[3] but it was only after the introduction of fractal geometry[4] that they were extensively analyzed in terms of scaling concepts. The simplest model, called "ballistic deposition," considers, in its "strip" two-dimensional version, a basal horizontal line of length L [the generalization to d dimensions considers a $(d-1)$-dimensional hypercube of edge L] on which particles are deposited, one after another, along randomly positioned vertical trajectories. Particles become part of the deposit at their positions of first contact (nearest-neighbor contact when on a lattice). This model has been extensively studied both on[5] and off lattice.[6] To analyze its surface properties, the following scaling form has been proposed:[7]

$$\sigma \sim L^{\alpha} f(h/L^{\alpha/\beta}), \qquad (1)$$

where h and σ are, respectively, the height of the deposit and the thickness of its surface. The scaling function $f(x)$ satisfies $f(x) \rightarrow$ const when $x \rightarrow \infty$ and $f(x) \sim x^{\beta}$ when $x \rightarrow 0$. Hence, the scaling behavior of σ is different with L for large h, $\sigma \sim L^{\alpha}$, than with h for large L, $\sigma \sim h^{\beta}$. The most accurate numerical estimates[4] of α and β, in two dimensions, are very close to $\alpha=\frac{1}{2}$ and $\beta=\frac{1}{3}$. Realistic extensions of this model were considered in which possible surface diffusion,[8] or particle restructuring,[6] is included. In particular, when a complete restructuring is considered, i.e., when the particles are allowed to slide on the surface until they reach the nearest local minimum, it is found that the scaling form (1) is still valid, but with a different β exponent, $\beta=\frac{1}{4}$, while α remains equal to $\frac{1}{2}$.[6]

It is now generally believed that such models are discrete versions of the continuous model introduced by Edwards and Wilkinson[8] and subsequently modified by Kardar, Parisi, and Zhang.[9] These authors describe the growing surface using a stochastic Burgers equation:

$$\frac{\partial h(\mathbf{r})}{\partial t} = v + \nu \Delta h(\mathbf{r}) + D\eta(\mathbf{r}) + \lambda |\nabla h(\mathbf{r})|^2 . \qquad (2)$$

In this expression, $h(\mathbf{r})$ is the vertical coordinate of a surface point whose other $(d-1)$ coordinates are described by $\mathbf{r}$; v is a constant proportional to the bulk compacity which can be dropped as far as only surface properties are concerned; the Laplacian term describes surface-tension effects and favors surface smoothing; $\eta(\mathbf{r})$ is a Gaussian random variable with zero mean which describes the noise; and the fourth (nonlinear) term, which has been first introduced by Kardar, Parisi, and Zhang,[9] describes the lateral growth of the surface. In two dimensions, it has been shown[10] that, without the nonlinear term, the solution of the Burgers equation follows the scaling *Ansatz* (1) with $\alpha=\frac{1}{2}$ and $\beta=\frac{1}{4}$, while, when the nonlinear term is included, the exponent β is changed into $\beta=\frac{1}{3}$. This is perfectly consistent with the results of numerical simulations since one can argue that a complete restructuring kills lateral growth and favors the Laplacian term.

The investigations in higher dimensions, both analytical and numerical, are presently very active. Kardar, Parisi, and Zhang[9] pointed out that $d=3$ must be a critical dimension above which the scaling of the full equation (2) should change. Recently, Halpin-Healy,[10] using nonlinear renormalization-group techniques, was able to make some more precise predictions. The behavior of (2) is governed by the strength of the reduced coupling constant $\bar{\lambda}=\lambda D/\nu^{3/2}$. For $d<3$ strong coupling should prevail for all $\bar{\lambda} \neq 0$ while for $d>3$, there should be, when increasing $\bar{\lambda}$, a transition between a weak-coupling and a strong-coupling phase, this transition becoming a mean-field type above $d_c=5$. No prediction is done for $d=3$, but one might expect some interesting marginal behavior. These predictions are in contradiction with the hypothesis of "superuniversality," i.e., growth exponents independent of spatial dimensionality, formulated earlier.[11]

It is of great importance to test numerically if the predictions of Halpin-Healy are observed in discrete models. We know about two very recent numerical works able to recover a transition in $d=3$ using modified ballistic models.[12,13] In the work by Amar and Family,[12] the connection with the Burgers equation is not fully transparent, while in the work by Yan, Kessler, and Sander (YKS),[13] an *ad hoc* parameter p is introduced whose effect is to smooth the surface exactly as does the Laplacian term in (2). Our method, which consists of interpolating directly between the nonrestructured and the completely restructured ballistic model by considering a random binary mixture of particles that slide or stick to the deposit upon contact, although very close, appears to be more powerful than that of YKS since it can be the subject of off-lattice extensions as well as interesting experimental realizations. Moreover, it allows us to analyze the surface-roughening transition through the bulk properties of the deposit. We are able to show that the transition is characterized by a singularity in the compacity-versus-concentration curve, which is very weak for $d=3$ and stronger for $d=4$ and which is accompanied by a peculiar percolation transition in the cross section of the bulk.

The present model is built on a d-dimensional simple cubic lattice, the base being a $(d-1)$-dimensional hypercube, H_{d-1}, perpendicular to the vertical direction. Particles are deposited one after another. After n particles have been deposited, the surface is defined by the integer function $h(i,n)$, where $i\in H_{d-1}$ defines a "column." One starts with a fully occupied base, i.e., with $h(i,L^{d-1})=1$ for all i. To deposit the $(n+1)$th particle $(n>L^{d-1})$ one proceeds as follows. A column i_0 is chosen at random in H^{d-1} to define the lateral position of its trajectory. Then, if a random variable (uniformly distributed between 0 and 1) is smaller than c, the particle is a "sticky" particle, otherwise it is a "sliding" particle. A sticky particle is deposited in column i_0 at $h_m=\max_j[h(i_0,n)+1,h(j,n)]$, where j runs over the $2(d-1)$ nearest neighbors of i_0 and H_{d-1} (periodic boundary conditions are considered at the edges of H_{d-1}). Thus, in that case, one sets $h(i,n+1)=h(i,n)$ for all i, except $h(i_0,n+1)=h_m$. A sliding particle, instead, follows the path of steepest descent on the surface, jumping from column i_0 to column $i_1,i_2,\ldots,i_p$ according to the rule that if $\min_j h(j,n)<[h(i_q,n)]$, i_{q+1} is the j value, or is chosen at random among the j values, realizing the minimum. The process stops when $\min_j[h(j,n)]\geq h(i_p,n)$ and the particle is then deposited in column i_p, i.e., one sets $h(i,n+1)=h(i,n)$, for all i, except $h(i_p,n+1)=h(i_p,n)+1$. Note that a sticky particle may leave some holes in the bulk, while a sliding particle cannot. Moreover, according to the rules, once created, a hole can never be filled, even by a sliding particle.

Our model interpolates between the completely restructured ballistic model, for $c=0$, with a compacity equal to 1 (no holes) to the plain ballistic model, for $c=1$, with a compacity lower than 1. At each step n of the deposition process we are able to calculate the mean height of the deposit, h, its compacity, ρ, and the thickness of its surface, σ, using the following formulas:

$$h=\frac{1}{L^{d-1}}\sum_i h(i,n)\,, \tag{3a}$$

$$\rho=\frac{n}{L^{d-1}h}\,, \tag{3b}$$

$$\sigma^2=\frac{1}{L^{d-1}}\sum_i[h(i,n)-h]^2\,. \tag{3c}$$

In our calculations, we have grown deposits of modest sizes, but we have systematically averaged our results over many independent runs to improve the statistics and understand clearly the size effects. In this Letter we present preliminary results, mainly to demonstrate the existence of a transition in $d=3$ and 4 and to show its manifestation in the bulk. We have considered L values up to $L_{\max}=128$, 64, and 32 in $d=2$, 3, and 4, respectively, and, to estimate the large-h saturation values of σ and ρ, we have grown deposits of height $h=64L$ and averaged the results over ten runs. Other calculations have been done to estimate the exponent β and will be reported elsewhere together with further results.

In Fig. 1, we have reported the saturated values of σ as a function of L for different c values (log-log plots). While for $d=2$ the curves are all roughly parallel and consistent with $\alpha=\frac{1}{2}$, for $d=3$ and 4 there is a clear threshold, c_s, at which an abrupt change of slope occurs. Below c_s, σ seems to saturate to a finite value when increasing L, while just above c_s, one observes a linear behavior for $\log\sigma$ vs $\log L$ up to the largest available size. Although the saturation is more evident for $d=4$, we think both results for $d=3$ and 4 below c_s are consistent with the weak-coupling logarithmic $(\alpha=0)$ behavior predicted by Edwards and Wilkinson.[8] From the slope of the curves just above the threshold, one obtains the estimates $\alpha=0.39\pm0.05$ and 0.34 ± 0.05, for $d=3$ and 4, respectively. These values are perfectly consistent with the result $\alpha=2/(d+2)$ of Kim and Kosterlitz;[14] however, due to our large error bars, one cannot completely exclude the alternative prediction $\alpha=1/d$ of Wolf and Kertész.[15] Far above the threshold, one obtains a lower slope. However, since one can reasonably assume that there should be no crossing between curves of different c values, this effect is certainly due to finite-size corrections and, for very large L, one should recover the same α exponent (we have tested this is not due to an underes-

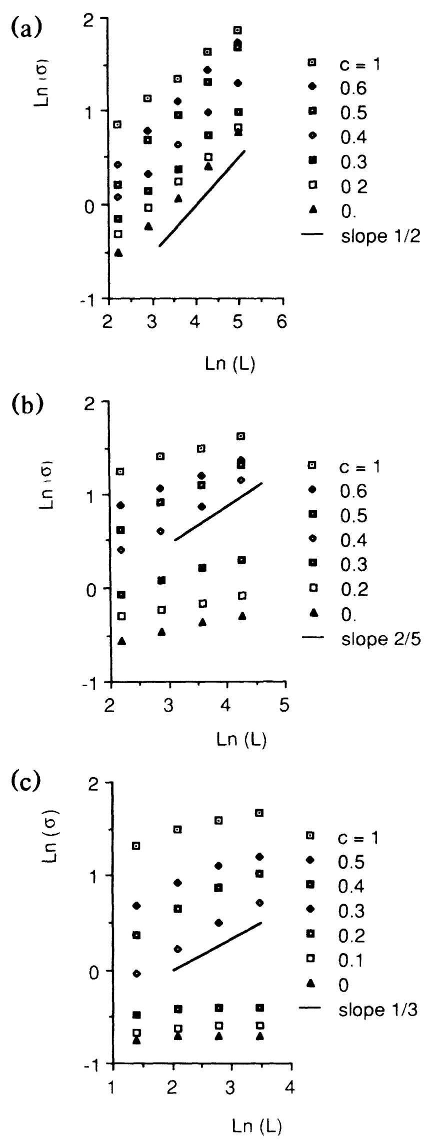

FIG. 1. Large-h saturated value of σ vs L (log-log plot) for different values of c. Cases (a), (b), and (c) correspond to $d=2$, 3, and 4, respectively.

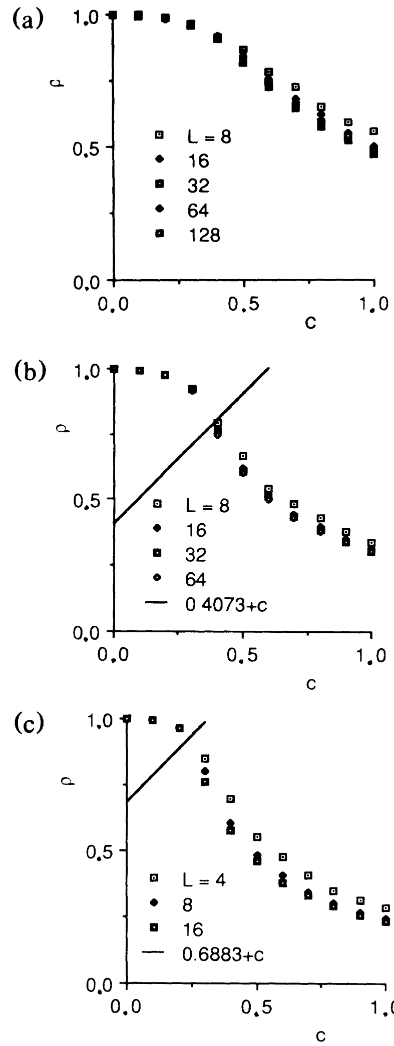

FIG. 2. Large-L saturated value of the bulk compacity, ρ, as a function of c. Cases (a), (b), and (c) correspond to $d=2$, 3, and 4, respectively. The line corresponds to the equation $\rho=c+1-c_p$, where c_p is the concentration threshold for site percolation on a $(d-1)$-hypercubic lattice ($c_p=0.5927$ and 0.3117, for $d-1=2$ and 3, respectively).

timation of the saturated σ value for large L and c). Thus the apparent linear behavior observed for large c might be followed by a change of slope for larger-L values.

In Fig. 2, we report the estimated large-h values of the bulk compacity as a function of c. While the curves for $d=2$ do not reveal any peculiar behavior, the curves for $d=3$ and 4 exhibit a sigmoidal shape which become more and more marked with increasing L. From a more quantitative analysis, which will be reported elsewhere, it appears that the maximum value of $\ln(\partial\rho/\partial c)$ increases linearly with $\ln L$ for $d=3$ and 4. However, for $d=3$, this increase is quite small and this might be the signature of a marginal behavior. Furthermore, when considering, for large h and L, a $(d-1)$-dimensional horizontal cut of the deposit, one observes that c_s corresponds to the site percolation threshold of the ensemble (sticky particles and holes). To demonstrate this more quantitatively, we have reported in Figs. 2(b) and 2(c) the straight line of the equation $\rho=1-c_p+c$, obtained when equating $c+1-\rho$, concentration of sticky particles and holes, and c_p, threshold for site percolation on a $(d-1)$-dimensional hypercubic lattice.[16] This line cuts the extrapolated curve exactly in the range where lies the expected c_s value, which can be more precisely estimated to be $c_s=0.37\pm0.01$ and 0.26 ± 0.01, for $d=3$ and 4, respectively. This result provides a very simple image of the roughening transition. Knowing that a hole in the bulk is always located below a sticky particle, the transition corresponds to the appearance of an infinite connected cluster of sticky particles when the surface is seen from the top. Hence, while below the threshold, a sticky particle most probably falls in a smooth "valley" of sliding particles; above the threshold, it sticks with a finite probability to the rough infinite cluster of sticky particles. It is interesting to notice that this percolation transition does not involve the vertical direction (i.e., time) and thus we think no trivial link between the deposition growth indices and the exponents of $d-1$ percolation should be expected.

In summary, using a very simple ballistic model which considers a mixture of sticky and sliding particles, we have given evidence for a roughening transition in $d=3$ and 4. In addition, we have shown that this transition is accompanied by a phase transition in the bulk of the deposit, characterized by a singularity in its compacity-versus-concentration curve and corresponding to a $(d-1)$-percolation transition. Much more numerical work is needed on this model to make the present results more precise, especially in the vicinity of the transition, and this will be the subject of further studies. Other trivial, but realistic, extensions are in progress, where sliding particles may fill the holes, or can be stopped by sticky particles of the deposit, etc. Moreover, one should study off-lattice analogs of these models, for example, by modifying the existing three-dimensional off-lattice model with restructuring.[17] Although the exponents will be difficult to estimate, the singularity in the compacity, however, should show up from a finite-size analysis. These models also suggest very simple practical realizations and we hope that there will soon appear some experimental evidence for the $d=3$ transition.

We thank R. Botet for discussions. Numerical calculations were done at CIRCE (Centre Inter-Régional de Calcul Electronique), Orsay, France.

[1]F. Family and D. P. Landau, *Kinetics of Aggregation and Gelation* (North-Holland, Amsterdam, 1984); H. E. Stanley and N. Ostrowski, *On Growth and Forms, a Modern View* (Martinus Nijhoff, Kluwer Academic, Boston, 1985); R. Jullien and R. Botet, *Aggregation and Fractal Aggregates* (World Scientific, Singapore, 1987).

[2]R. Jullien, L. Peliti, R. Rammal, and N. Boccara, *Universalities in Condensed Matter,* Proceedings in Physics Vol. 32 (Springer-Verlag, Berlin, 1988).

[3]M. J. Vold, J. Colloid Interface Sci. **14**, 168 (1959); J. Phys. Chem. **63**, 1608 (1959); **64**, 1616 (1960).

[4]B. B. Mandelbrot, *The Fractal Geometry of Nature* (Freeman, San Francisco, CA, 1982).

[5]P. Meakin, P. Ramanlal, L. M. Sander, and R. C. Ball, Phys. Rev. A **34**, 5081 (1986).

[6]F. Family, J. Phys. A **19**, L441 (1986).

[7]F. Family and T. Vicsek, J. Phys. A **18**, L75 (1985).

[8]S. F. Edwards and D. R. Wilkinson, Proc. Roy. Soc. London A **381**, 17 (1982).

[9]M. Kardar, G. Parisi, and Y. C. Zhang, Phys. Rev. Lett. **56**, 889 (1986).

[10]T. Halpin-Healy, Phys. Rev. Lett. **62**, 442 (1989); (to be published).

[11]M. Kardar and Y. C. Zhang, Phys. Rev. Lett. **58**, 2087 (1987); A. J. McKane and M. A. Moore, Phys. Rev. Lett. **60**, 527 (1988).

[12]J. G. Amar and F. Family (to be published).

[13]H. Yan, D. Kessler, and L. M. Sander, Phys. Rev. Lett. **64**, 926 (1990).

[14]J. M. Kim and J. M. Kosterlitz, Phys. Rev. Lett. **62**, 2289 (1989).

[15]D. E. Wolf and J. Kertész, Europhys. Lett. **4**, 1385 (1987); J. Kertész and D. E. Wolf (to be published).

[16]D. Stauffer, *Introduction to Percolation Theory* (Taylor and Francis, London, 1985).

[17]R. Jullien and P. Meakin, Europhys. Lett. **4**, 1385 (1987); and **6**, 629 (1988).