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Simulations of deposition growth models in various dimensions: The possible importance of overhangs

David Y. K. Ko and Flavio Seno
Department of Physics, University of Oxford, 1 Keble Road, Oxford, OX1 3NP, United Kingdom
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We present simulation results of deposition growth of surfaces in two, three, and four dimensions for ballistic deposition where overhangs are present, and for restricted solid on solid deposition where there are no overhangs. The values of the scaling exponents for the two models are found to be different, suggesting that they belong to different universality classes.

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The deposition growth of surfaces [1] has been a subject of long continual theoretical and experimental interest [2] due to its relevance to nonequilibrium processes in general as well as its possible role in surface technology. The profile of the deposited surface gradually roughens under the stochastic accumulation of particles, and early simulations by Family and Vicsek [3] suggested that the surface roughness exhibits a dynamical scaling behavior. That is, the height-height correlation function $G(r-r',t)=\langle[h(r,t)-h(r',t)]^2\rangle^{1/2}$ scales with time t and separation $\ell=|r-r'|$ as

$$G(\ell,t)\sim\ell^{\alpha} f(t/\ell^{z}). \quad (1)$$

$h(r,t)$ is the height of the surface at position r and at time t. The dynamical scaling behavior is characterized by the roughness exponent α and the dynamical exponent β, with $z=\alpha/\beta$. The scaling function $f(x)$ behaves as $f(x)=x^{\beta}$ for $x\ll 1$ and $f(x)=$ const for $x\gg 1$. Thus the surface roughness grows as $G(t)\sim t^{\beta}$ initially, independent of size, and for a given size, ℓ, the roughness saturates after a sufficiently long time such that $G(\ell)$ scales with ℓ only as $G(\ell)\sim\ell^{\alpha}$.

Numerous simulations in a variety of growth models [4–7] have since confirmed the hypothesis of dynamical scaling, including models which allow overhangs to form and models where overhangs are not allowed. An overhang is formed when a particle sticks at a position higher than the height of the surface at that point, such that the space below the particle is not filled. Simulations of the restricted solid on solid model [10,11], where incoming particles fall directly onto the surface such that no overhangs can form, and may only stick at a site if the resulting nearest neighbor height differences are less than some predetermined value, have led to a further consensus that the value of the scaling corresponds to that of the Kardar-Parisi-Zhang equation [12],

$$\frac{\partial h}{\partial t}=\nu\,\nabla^2 h+\frac{\lambda}{2}(\nabla h)^2+\eta,$$

where η is a random variable. This equation is believed to be a continuum description of deposition growth, and was derived by assuming that the surface grows uniformly in the direction of the local normal. The exponents obtained are exact in two dimensions [12], and numerically determined in higher dimensions [8,9].

Results from simulations of the ballistic deposition model [13] where incoming particles stick at the first point of contact and thus allow overhangs are more controversial. At present there is no clear consensus as to whether or not this system belongs to the same universality class as that described by the Kardar-Parisi-Zhang equation [14], or whether the presence of overhangs leads to a different set of scaling exponents. Early results by Meakin *et al.* gave $\alpha=0.47$ and $\beta=0.331$ in two dimensions, and $\alpha=0.33$ and $\beta=0.24$ in three dimensions, in agreement with Kim and Kosterlitz's approximate formula [5] of $\alpha=2/(d+2)$ and $\beta=1/(d+1)$ for the Kardar-Parisi-Zhang equation. More recent results suggest that the values of the scaling exponents may, in fact, be different. Baiod *et al.* [15] obtained $\beta=1/3$ in two dimensions and $\alpha=0.3$ and $\beta=0.22$ in three dimensions; off-lattice simulations have also given $\beta=0.343$ in two dimensions [16], but a clear scaling behavior was not observed in three dimensions [17].

In this paper, we report results of simulations of ballistic deposition and restricted solid on solid growth. We find that the values of the scaling exponents for the ballistic deposition model are different from those of the restricted solid on solid model. A summary of our results is given in Table I.

We also find that while on-lattice simulations give excellent scaling behavior for the restricted solid on solid model, the same is not true for ballistic deposition. Quasi-off-lattice simulations were therefore carried out for the ballistic deposition model. Namely, each axis of a surface of size L^{d-1} particle diameters is divided into nL points such that incoming particles can be centered on any one of these points. For

TABLE I. Scaling exponents obtained from our simulations.

Dimension	Ballistic deposition			Restricted solid on solid		
d	α	β	z	α	β	z
2	0.45	0.32	1.40	0.50	0.33	1.50
3	0.26	0.21	1.24	0.40	0.25	1.60
4	~0.12			0.29	0.18	1.61

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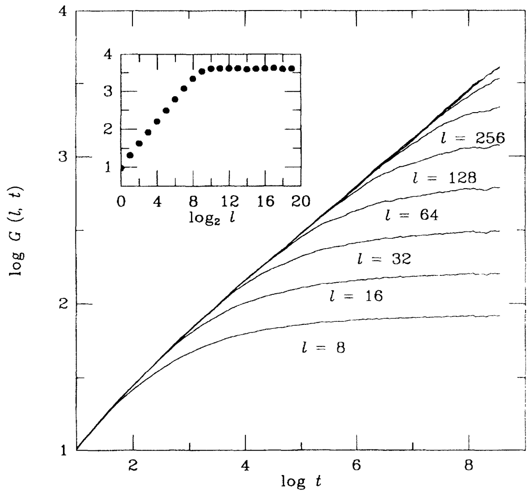

FIG. 1. Ballistic deposition for two dimensions. The inset shows the plot of $\ln G(\ell,t)$ versus $\log_2 \ell$ at the end of the simulation.

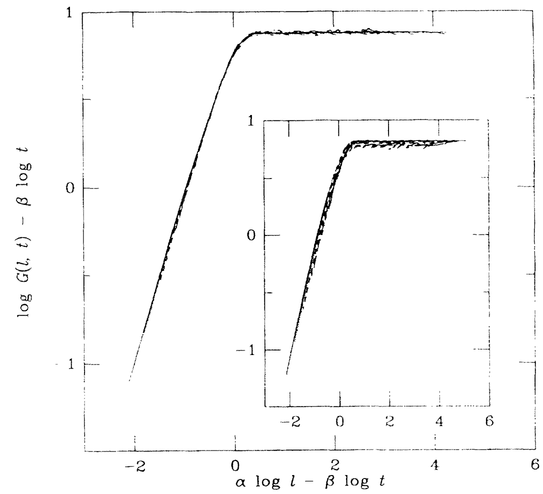

FIG. 2. Collapsed data for two dimensional ballistic deposition simulation, with $\alpha=0.45$ and $\beta=0.32$. The data used range from $\ell=2^2$ to 2^{19}. The inset shows the collapse obtained with the exponents obtained for the restricted solid on solid model. Natural logarithms are used for the collapse.

n large, the surface approaches a continuum, and for $n=1$, we recover the on-lattice model. The height of the surface at a position r is defined to be the height of a new particle if it fell onto the surface at r. We found that $n=3$ is sufficient to give a good scaling behavior, and no differences were found in the results with $n=$ 5, 7, and 10. We performed simulations in two, three, and four dimensions for both models and the simulations are run until the equivalent of at least 2000 layers of atoms have been deposited. The total number of particles deposited in each simulation is over 2×10^9. The minimum time required for each run is 24 CPU hours on a DEC Alpha 400 workstation. To obtain good statistics, averages over up to ten runs were often needed. We note that our estimates of the scaling exponents are obtained "by eye." That is, when a set of scaling exponent values were found which gave the best data collapse, values close to it were tried until the collapse became poor. The errors quoted therefore correspond to the range of values where no appreciable difference in the quality of the collapse was observed. This method is used as we did not want to prejudice any result by fitting the collapsed data to some arbitary functional form, and the range of data used is large enough for the data collapse to be sufficiently sensitive to the particular values of the exponents used.

In Fig. 1, the correlation function $G(\ell,t)$ for a two dimensional ballistic deposition simulation is plotted versus time in a log-log plot. The largest system size considered is $\ell=2^{20}$. For the larger values of ℓ, the roughness has not saturated within the time scale of the simulation. In the dynamical scaling region, we see a clear power law behavior, $G(t)\sim t^{\beta}$. Also shown in the inset is a plot of $\ln G(\ell,t)$ versus $\log_2 \ell$ for the data at the end of our simulation. For the smaller sizes where saturation has been reached, we also find a roughly linear dependence of $\ln G$ on $\log_2 \ell$ in agreement with the predictions of dynamical scaling.

Direct extrapolation of the scaling exponents from the gradients in the log-log plots turned out to be difficult because crossover effects due to the transition from the dynamical scaling regime to the saturated scaling regime introduce significant corrections. Instead, by rewriting Eq. (1) as

$$\ln G(\ell,t)-\beta \ln t=F(\alpha \ln \ell-\beta \ln t), \tag{2}$$

we can obtain good estimates of the dynamical and roughness exponents by collapsing our data for all sizes and all times considered. This, in fact, provides a way of checking also whether the data correspond to just one scaling regime, or whether there is also a crossover between different universality classes with different scaling exponents. We note that the surface roughness during the initial few time steps is strongly influenced by transient effects, and have been discarded in the data collapse.

The collapsed data for the two dimensional ballistic deposition result is shown in Fig. 2. Data for ℓ ranging from 2^2 to 2^{19} are used in the plot, with over 6×10^9 particles deposited. The values of the exponents used are $\alpha=0.45$ and $\beta=0.32$. We have also carried out simulations of the restricted solid on solid model in two dimensions, and found that $\alpha=0.50$ and $\beta=0.33$, in agreement with the results of previous simulations.

The collapsed data for the three dimensional simulations are shown in Fig. 3. The upper diagram is for the restricted solid on solid model. The size of the system considered is $2^{10}\times 2^{10}$, and over 2×10^9 particles were deposited in a run. The data presented represent the average over seven independent runs, and include values for ℓ ranging from 2^2 to 2^9. The values of the scaling exponents obtained in this case are $\alpha=0.40$ and $\beta=0.25$. This is in agreement with the approximate formula of Kim and Kosterlitz [5], but the value of β obtained is greater by 0.01 than that observed more recently by Ala-Nissila *et al.* [11].

Ballistic deposition simulations in three dimensions are also carried out for systems with size equal to $2^{10}\times 2^{10}$ particle diameters, with three subdivisions per particle diameter. The collapsed data are shown in the lower diagram of Fig. 3.

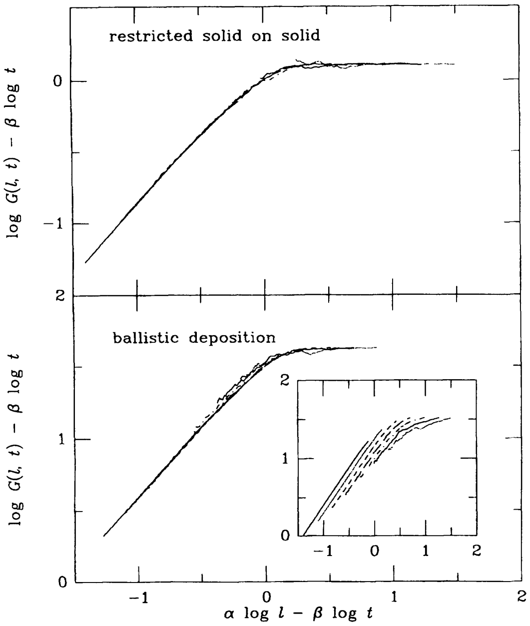

FIG. 3. Collapsed data for the three dimensional restricted solid on solid simulation (upper diagram), and the ballistic deposition simulation (lower diagram) for $\ell = 2^2$ to 2^9. The inset in the lower diagram shows the collapse obtained if the exponents obtained from the restricted solid on solid model were used instead. Natural logarithms are used for the collapse.

Again, over 2×10^9 particles were deposited per run, and the results presented represent the average over ten runs with data for $\ell = 2^2$ to 2^9 used in the data collapse. The simulations were also carried out with seven subdivisions per particle diameter and no difference was found. The values of the scaling exponents in this case are $\alpha = 0.26$ and $\beta = 0.21$, significantly lower than the corresponding values for the restricted solid on solid model.

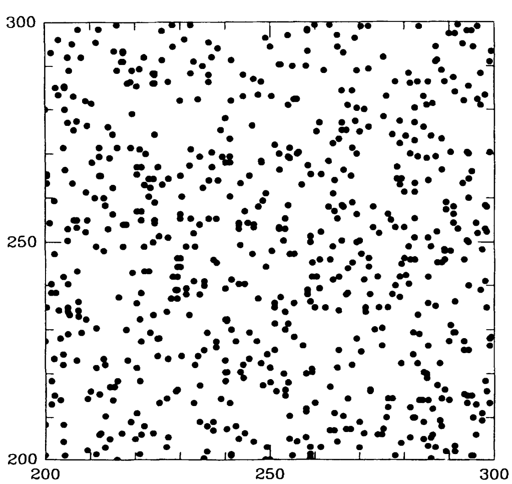

FIG. 4. A cross section of ballistic deposition growth in three dimensions taken at a height of 200 particle diameters. The length of the horizontal and vertical axis corresponds to 100 particle diameters.

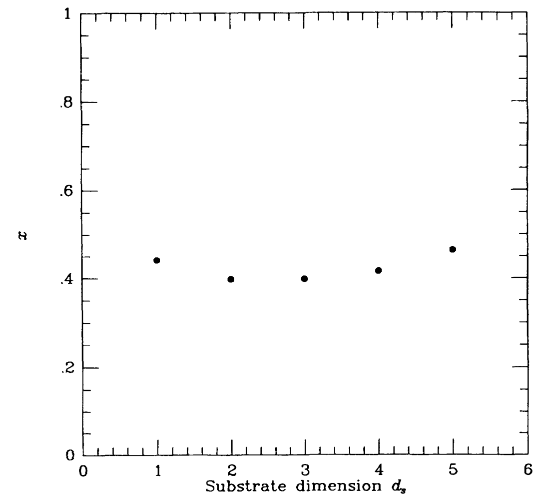

FIG. 5. The fraction x of sites occupied along a substrate dimension versus the substrate dimension.

We have also carried out simulations in higher dimensions for both models. However, due to computational difficulties, we are restricted to relatively small sizes. For the ballistic deposition model the largest size possible in four dimensions or higher is still too small for the dynamical scaling regime to be observed. Estimates of the roughness exponent in four dimensions, however, give a value of $\alpha \approx 0.12$. The uncertainty in this case is due to strong fluctuations in the roughness as a result of the small system size, and the number of runs required to obtain better statistics is prohibitively large. For the restricted solid on solid model, the fluctuations are smaller even in four dimensions and we have been able to obtain reliable values for both the dynamical and the roughness exponents. These are $\alpha = 0.29$ and $\beta = 0.18$, in good agreement with those obtained by Ala-Nissila *et al.* [11]. Again, in accordance with the trend observed in lower dimensions, the exponent of the ballistic deposition model is lower than that of the restricted solid on solid model.

We have found that variations in the value of either α or β by as little as 0.01 are sufficient to give clear deterioration of the data collapse plots. The values we present are therefore accurate to the figures quoted. The most important implication of this is that, from our results, the dynamical scaling behavior of the ballistic deposition model and the restricted solid on solid model belong to different universality classes. We have shown in the insets to Figs. 2 and 3 what happens when we try to collapse the ballistic deposition data with the exponents obtained from the corresponding restricted solid on solid simulations. It is clear from the diagrams that even in two dimensions, where the differences between the values of the scaling exponents for the ballistic deposition model and those of the restricted solid on solid model are apparently small, a satisfactory data collapse cannot be obtained. In view of the belief that the dynamics of the restricted solid on solid model corresponds to that of the Kardar-Parisi-Zhang equation, our results would therefore further suggest that the Kardar-Parisi-Zhang equation is not appropriate in describing deposition growth in situations where overhangs are dominant. Indeed, our values of the scaling exponents for the ballistic deposition model in two, three, and four dimensions lie outside the range of the values for the Kardar-Parisi-Zhang exponents [12,8,9].

We have also tried to examine the structure of the solid formed by growth under ballistic deposition conditions. Figure 4 shows a cross section of the bulk formed in a three dimensional ballistic deposition simulation. The cross section corresponds to a height of 200 particle diameters from the substrate, and is taken after all the particles at this height are covered. The cross section shown corresponds to an area of 100×100 particle diameters. We find that there are very few connected lines, and no connected rings in the cross section. In addition, we have calculated the fraction of sites, x, which are occupied in a linear direction from the average density, ρ. For a d_s dimensional surface, the density is given by $\rho = x^{d_s}$. In Fig. 5 a plot of x versus substrate dimension is shown. The results indicate that of order 0.4 of the sites along a line on the surface are occupied in all dimensions. This, together with the cross section plot, corroborates the idea that particles grow on the edges of overhangs, and almost immediately branch off to form a complex treelike structure.

In summary, we have found that the presence of overhangs is an important factor in determining the scaling properties of deposition growth. In a model such as ballistic deposition, overhangs will form when the local surface gradient exceeds a critical value corresponding to the presence of a sharp step in the surface profile. In such a situation, the next particle will stick to increase the lateral size of the overhang region rather than to reduce the surface gradient by falling to the lower surface. Thus, as overhangs begin to form, they will tend to increase the lateral correlation at a fast rate, and the surface will no longer grow in the direction of its local gradient. The result may be an anisotropic growth which when coarse grained leads to broader and flatter structures. Although such a picture can give a behavior consistent with the results of our simulations, the search for a proper theory for deposition growth in the presence of overhangs remains an important challenge.

Note added. Since submission we have received a copy of unpublished work from Cieplak, Maritan, and Banavar [18] in which they reported the possible significance of overhangs in some related problems.

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