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LETTER TO THE EDITOR

Concentration effects in the off-lattice random ballistic deposition model

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Abstract. The influence of a finite concentration of particles in random ballistic deposition is studied using a simple two-dimensional off-lattice model. Discs are initially randomly placed, without overlap, in a rectangle. Then they are allowed to fall along the vertical direction and they stop as soon as they contact another disk or the bottom of the rectangle. This process leads to uniform deposits whose density has been estimated for various initial densities. At the 'jamming' threshold (when no more discs can be added to the initial configuration), it is found that the density difference between the deposit and the initial configuration reaches a well defined non-zero value. Moreover, the exponent β, which shows how the surface thickness grows with the height of the deposit, is shown to stay very close to $\frac{1}{3}$, independently of the initial concentration, up to jamming.

The deposition of particles onto surfaces is a process of considerable scientific interest with a broad range of practical applications. The simulation of such processes was pioneered by Vold [1] almost 30 years ago. More recently, interest has developed in ballistic deposition models as a result of the general interest in non-equilibrium growth and aggregation processes [2] which was initiated by the introduction of a simple model for diffusion-limited aggregation by Witten and Sander [3]. It has been found that the deposit formed by random ballistic deposition has a compact structure (uniform on all but very short length scales) with a well defined density, while its surface exhibits a self-affine [4, 5] fractal geometry which can be described in terms of the scaling form [4]:

$$\xi = l^{\alpha} f(h/l^{\alpha/\beta}) \tag{1}$$

where ξ is the surface thickness, h is the mean height of the deposit and l is the lateral size of the system (periodic boundary conditions are used in almost all the simulations). The scaling function $f(x)$ tends to a constant value when x tends to infinity and has the form x^{β} when x tends to zero. This implies that ξ grows as l^{α} for $h \gg l^{\alpha/\beta}$ and as h^{β} for $l^{\alpha/\beta} \gg h$. In two dimensions lattice simulations give $\alpha = \frac{1}{2}$ and β about $\frac{1}{3}$ [4, 6] and the theoretical work of Kardar *et al* [7] indicates that $\alpha = \frac{1}{2}$ and $\beta = \frac{1}{3}$, exactly.

In such simulations, the limit of a very low particle concentration in the incoming flux was implicitly assumed since particles were added to the deposit one at a time. The effect of finite concentration has already been studied using on lattice ballistic models with [8] or without [9] restructuring. When restructuring is allowed, it has been shown that the exponent β is changed from $\frac{1}{3}$ to $\frac{1}{4}$ [8]. It must be noticed that lattice models cannot lead to realistic structures on short length scales and ignore all

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the interesting features occurring at high concentration due to the natural limits of randomly packing spherical particles.

In this letter, we study the influence of a finite concentration of particles in the random ballistic deposition process using a simple two-dimensional off-lattice model without restructuring. Particles are considered as hard discs of radius r_0 whose centres are initially randomly placed, without overlap, within a rectangle of size l in the horizontal direction and h_m in the vertical direction. To diminish edge effects in the non-overlapping initial state, we have used periodic boundary conditions in both directions. The concentration, or the density,is here defined as being the relative coverage:

$$\rho = Ns_0/(lh_m) \tag{2}$$

where N is the total number of discs and $s_0 = \pi r_0^2$ their surface.

To build the initial configuration, we perform sequential trials. At each trial the coordinates for the centre of a new disc are chosen at random (with a uniform probability) between 0 and l and between 0 and h_m, respectively. If there is overlap with previous discs, the new disc is discarded and another trial is performed. This procedure corresponds exactly to the random sequential adsorption model [10, 11]. For this model, it has been shown that there exists a critical number of particles, corresponding to a critical value for the concentration, ρ_c, above which no more particles can be added to the initial configuration. At this 'jamming' threshold, it has been demonstrated [10] that the number of trials N_t necessary to obtain the density ρ diverges according to:

$$N_t \alpha (\rho_c - \rho)^{-2}. \tag{3}$$

In practice we have averaged all our results, including concentrations, over a large number of simulations N_s corresponding to different random initial configurations built with the same number of trials N_t. Thus, in a given simulation, the initial configuration is completed when the desired number of trials has been performed. Then the ballistic deposition process starts. In this process all particles are considered to have the same speed so that an iterative procedure can be used in which all the particles are sequentially visited in ascending order of their vertical coordinates. At the ith iteration, the selected particle is allowed to fall vertically until it reaches a position at which it either contacts the basal line or another, previously deposited, particle. The basal line is chosen to be the horizontal line of vertical coordinate $-r_0$ (it could have been any other horizontal line of smaller coordinate without changing the results). For some selected i values, the density profile of the bulk has been averaged over the N_s simulations. Also, for these i values, the height of the deposit h as well as the thickness of its surface ξ have been calculated as being the average and the standard deviation of the vertical coordinates z_i over N_s simulations:

$$\begin{aligned} h &= \langle z_i \rangle_s \\ \xi^2 &= \langle (z_i - h)^2 \rangle_s \end{aligned} \tag{4}$$

where $\langle \ldots \rangle_s$ denotes the average over the N_s simulations with the same N_t.

We found a linear variation of h with i, which is consistent with a uniform deposit. The bulk density has been then estimated from the plateau of the density profile for the last iteration and averaged over the N_s simulations.

In figure 1, we show the initial configuration as well as the final configuration (after the last iteration) for three typical simulations corresponding to different values of the initial concentration.

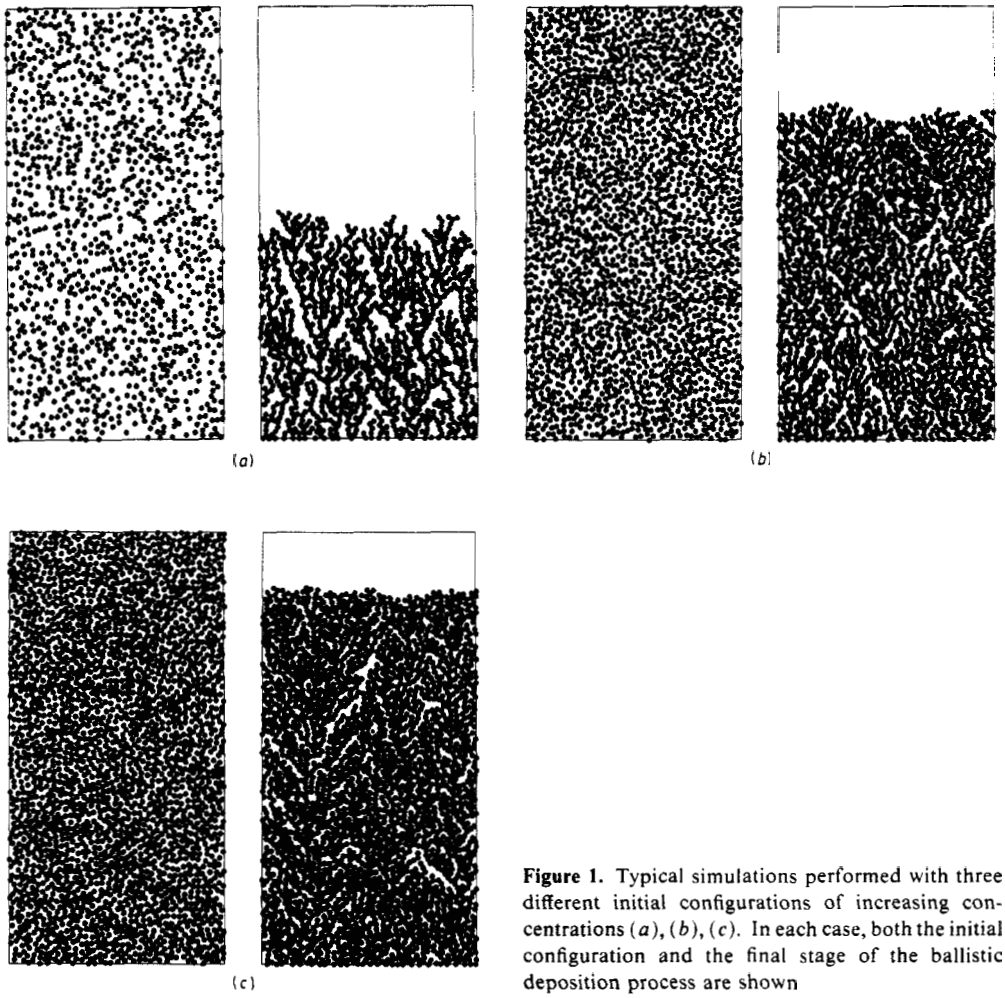

Figure 1. Typical simulations performed with three different initial configurations of increasing concentrations (*a*), (*b*), (*c*). In each case, both the initial configuration and the final stage of the ballistic deposition process are shown

To study the bulk and surface properties of the deposit, we have performed three series of calculations taking always $h_m = 4l$ but with three different values of l: $l = 16$, 32, 64. Here the unit of length is such that $r_0 = 0.708$, is slightly larger than $2^{1/2}$ (this is due to the fact that we use an underlying lattice with at most one particle centre per cell to locate particles near the selected particle). In each case we have averaged over $N_s = 500$ simulations and a sequence of N_t values has been chosen according to:

$$N_t = N_{t0} 2^j \qquad j = 1, 2, \ldots j_{max} \tag{5}$$

with $N_{t0} = lh_m/(16s_0)$ and $j_{max} = 13$, 13, 11 for $i = 16$, 32, 64, respectively. This choice ensures a quasilinear sequence of initial concentrations for small concentrations, far from jamming. As a general result we found that the size does not crucially affect the results and in the following we report the results obtained for $l = 32$ for which we were able to go closer to the jamming threshold.

The results for ρ_0 (initial concentration) and ρ_b (bulk concentration of the final deposit), have been reported as a function of $N_t^{-1/2}$ in figure 2. This figure clearly shows a linear dependance of both ρ_0 and ρ_b on $N_t^{-1/2}$. Using a least-squares fit of

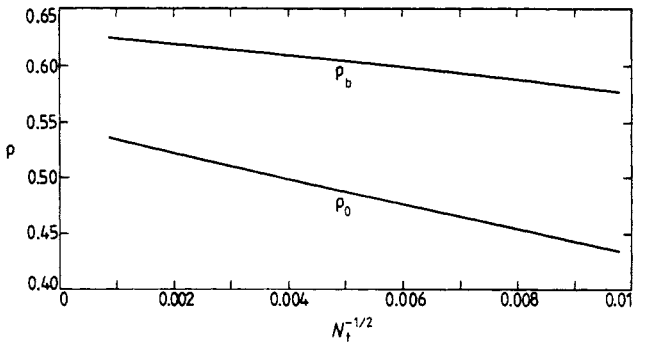

Figure 2. Density of the initial configuration, ρ_0, and density of the bulk, ρ_b, plotted as a function of $N_t^{-1/2}$. The results come from an average over 500 simulations performed in a rectangle of 32×128 with discs of radius 0.708.

the data, we obtain the following estimates at the jamming limit:

$$\rho_{0c} = 0.547 \pm 0.002$$

$$\rho_{bc} = 0.629 \pm 0.003.$$

The larger uncertainty on ρ_{bc} comes from the fact that ρ_b involves two averages: the average over the plateau of the bulk density for each iteration and the average over the N_s simulations. We have observed that these estimates are insensitive to l, in the chosen range of l values.

Our result for ρ_{0c} is consistent with the estimates already obtained by Feder [10] (0.547 ± 0.002) and by Tanemura [11] (0.5473 ± 0.0009) for the random sequential absorption model. When considering our results for the bulk density of the deposit it is interesting to observe that ρ_b, which is obviously always larger than ρ_0, varies also linearly with $N_t^{-1/2}$ near the jamming limit. Moreover the difference $\Delta\rho = \rho_b - \rho_0$ reaches a well defined non-zero value at $\rho_0 = \rho_{0c}$: this clearly shows the 'loose packing' character of the jammed configuration which here can be easily compacted by the effect of gravity.

Some typical results for ξ (surface thickness) as a function of h (height of the deposit) are depicted in figure 3, in the case $l = 32$. Similar qualitative results have

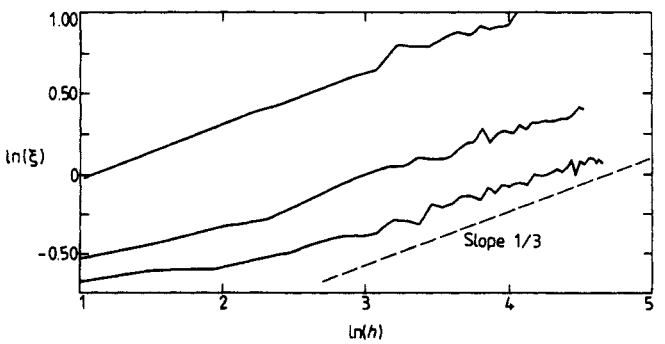

Figure 3. Surface thickness, ξ, of the surface as a function of the mean height of the deposit, h (log-log plot) for three different initial concentrations $\rho_0 = 0.2466$, 0.4344 and 0.5361. The results come from an average over 500 simulations performed in a rectangle of 32×128 with discs of radius 0.708.

been obtained for other l values. As expected, the surface thickness decreases when the initial concentration increases. However, it appears that when h becomes larger than a typical value h^*, a power law behaviour of the kind $\xi = h^\beta$ is recovered with $\beta = 0.30$, independently of ρ_0. This result is consistent with $\beta = \frac{1}{3}$ if one considers that saturation effects can be neglected (since our range of h values satisfies the condition $h \ll l^{\alpha/\beta}$). We have found no evidence for a diverging h^* when approaching jamming. Instead it seems that the curve $\xi(h)$ reaches a well defined limiting curve. At the jamming limit, $\xi(h^*)$ could correspond to some kind of mean distance between neighbouring discs in the jammed configuration.

In conclusion, it seems that in our off-lattice model, concentration effects do not affect the scaling behaviour of the surface thickness as has already been found in lattice models [8]. However, we have been able to show other interesting features in high concentrations which could not be revealed by lattice models. In particular we have found that the jammed configuration can simply be compactified by gravity effects. It would be interesting to extend this study in three dimensions and to consider some other initial configurations with higher concentrations. We could also include both concentration effects and restructuring as has been already done on the lattice [8]. We believe our study could be usefully compared with an experiment in which spheres, initially deposited into parallel horizontal plates, could be drifted by gravity after simply tilting the plates.

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