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LETTER TO THE EDITOR

Ballistic deposition with non-uniform deposition densities: singular density distributions

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Abstract. Ballistic aggregation and deposition with non-uniform deposition probability densities have been investigated. For the case of a singular power law, the density distributions can be described by the strength parameter α. Simple theoretical arguments and computer simulations indicate that $h \sim s^{\nu_\parallel}$ and $w \sim s^{\nu_\perp}$ where h is the cluster height, w is the cluster width and s is the cluster size. The exponents $\nu_\parallel$ and $\nu_\perp$ are given by $\nu_\parallel = (d-\alpha)/d$ and $\nu_\perp = 1/d$ where d is the dimensionality of the space in which ballistic aggregations are occurring.

Simple models for ballistic deposition processes in which particles are brought to a growing surface or aggregate via linear trajectories have been explored for more than 25 years (Vold 1959a, b). During the 1970s considerable interest developed in ballistic deposition models motivated by the need to obtain a better understanding of thin film deposition processes used to manufacture devices with unique optical, electronic, magnetic, tribological and mechanical properties (see for example Henderson *et al* 1974, Kim *et al* 1977, Dirks and Leamy 1977, Leamy and Dirks 1977, Leamy *et al* 1980). In recent years there has been a resurgence of interest in ballistic deposition and aggregation models, stimulated by the introduction of the diffusion-limited aggregation model by Witten and Sander (1981) which led to the investigation of a wide variety of non-equilibrium growth and aggregation models.

In all of the ballistic aggregation and deposition models investigated so far a random uniformly distributed flux of particles was assumed. These models lead to the formation of structures which are uniform on all but short length scales with self-affine fractal surfaces (see Family and Vicsek 1985, Meakin *et al* 1986, Kardar *et al* 1986, for example). Essentially uniform deposition is found in many important processes such as sedimentation and vapour deposition. However, it is also possible for particles to be transported by non-linear dynamic processes, chaotic flows, etc (Ottino *et al* 1988) which will, in general, lead to very non-uniform deposition density distributions. Here simple random deposition models are considered in which particles are deposited from one direction onto a growing cluster or deposit. In these models the deposition probability that a particle will follow a ballistic trajectory at a distance in the range X to $X+\delta X$ from a parallel vector passing through the origin is given by

$$P(X) \sim X^{-\alpha'} \delta X. \tag{1}$$

Consequently, the probability that a trajectory will pass within a distance l from the origin is given by

$$P(l) \sim l^{\alpha} \tag{2}$$

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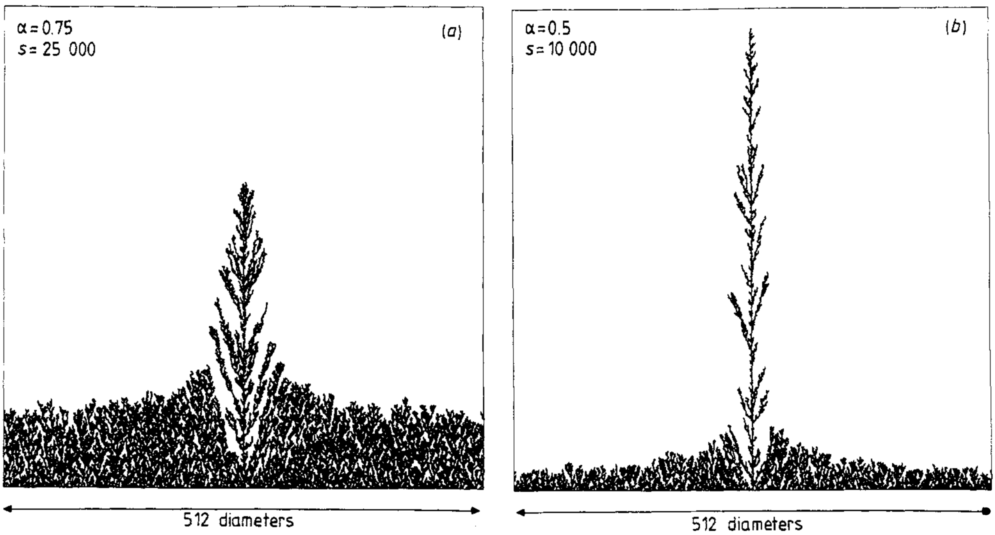
where the exponent α is given by

$$\alpha = d_s - \alpha' \tag{3}$$

where $d_s = d - 1$ and d is the dimensionality of the space in which the ballistic deposition or aggregation process is occurring (in a deposition process d_s is the dimensionality of the substrate).

Figure 1 shows results from small scale two-dimensional ($d = 2$, $d_s = 1$) off-lattice simulations in which particles of unit diameter were deposited one at a time at normal incidence to a linear substrate with a length (L) of 512 particle diameters. Apart from the fact that the deposition density at a distance X from the origin (at the centre of the substrate) is given by equation (2) the simulations are identical to off-lattice ballistic deposition simulations with a uniformly distributed random flux (Meakin *et al* 1986, Meakin 1987). Periodic boundary conditions were used in the lateral direction. It is



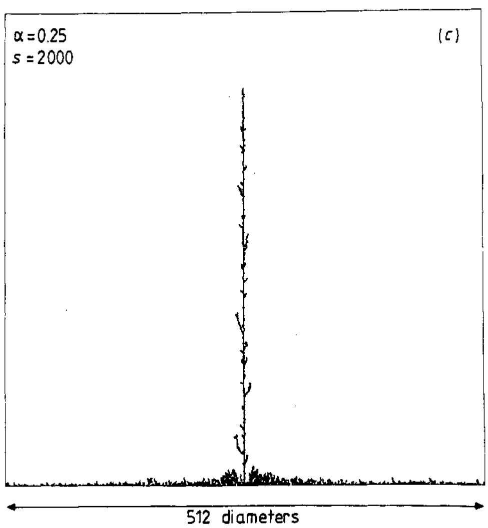


Figure 1. Two-dimensional off-lattice simulations of ballistic deposition onto a line with singularities of strength α ($\alpha = 0.75, 0.5$ and 0.25 in (a), (b) and (c) respectively).

apparent from figure 1 that the structure of the deposit is very similar to that found for a uniform particle deposition density except for positions near to the singularity in the deposition density at a position of $L/2$.

Since the structure of the 'tree' at $L/2$ does not depend on the more uniform part of the deposit at longer distances, simulations were also carried out in which a cluster was grown starting with a single 'particle' at the position of the singularity (figure 2). For the case $\alpha = 1$ ($\alpha' = 0$) this model corresponds to the 'rain' model (Bensimon *et al* 1984). For other values of α and α' the overall shape and internal structure of the clusters is quite different (figures 2(b–d)). To obtain a more quantitative characterisation of these clusters the dependence of the maximum height (h), the maximum width (w) and the height at which the cluster width is greatest ($h_2 = h_l + h_r$, see figure 3) on the cluster size s was measured. Clusters of size $s = 10^6$–10^7 were generated and results obtained from a number of simulations (typically several hundreds for $s = 10^6$ or several tens for $s = 10^7$). For example, figure 4 shows the dependence of the lengths (l) h, h_2 and w on the cluster size (number of particles) s. The results shown in figure 4 were obtained from 73 simulations in which clusters of size $s = 10^7$ were grown with $\alpha = 0.4$ ($\alpha' = 0.6$). In all cases the dependence of h and w on s can be represented very well by

$$h \sim s^{\nu_\parallel} \tag{4}$$

$$w \sim s^{\nu_\perp} \tag{5}$$

where $\nu_\parallel = (2-\alpha)/2$ and $\nu_\perp = 0.5$. The values obtained from the exponents $\nu_\parallel$ and $\nu_\perp$ are given in table 1. The statistical uncertainties are quite small ($\leqslant \pm 0.0001$). The dependence of cluster height at the maximum width on the cluster size can also be expressed in terms of a power law

$$h_2 \sim s^\eta \tag{6}$$

and the values obtained for the effective exponent η are given in table 1. The statistical uncertainties for η are much larger ($\leqslant \pm 0.005$).

The mean rates of growth of the cluster width (w) with increasing cluster size (s) are given by the probability that a particle will be deposited along a trajectory with an impact parameter of $w/2$ to $w/2 + d_0$ where d_0 is the particle diameter and w is the maximum difference for the x coordinates for any pair of particles in the deposit. From this it follows that

$$\mathrm{d}w/\mathrm{d}s \simeq (w^{\alpha-1} d_0)/(w^\alpha) \tag{7}$$

and that $w \sim s^{1/2}$. Similarly, the cluster height will grow if the deposited particle has an x coordinate close to that of the tip of the cluster near $x = 0$ and an estimate of this probability is given by

$$\mathrm{d}h/\mathrm{d}s \sim (d_0/w)^\alpha \tag{8}$$

or

$$\mathrm{d}h/\mathrm{d}s \sim s^{-\alpha/2} \tag{9}$$

which implies that

$$h \sim s^{(2-\alpha)/2}. \tag{10}$$

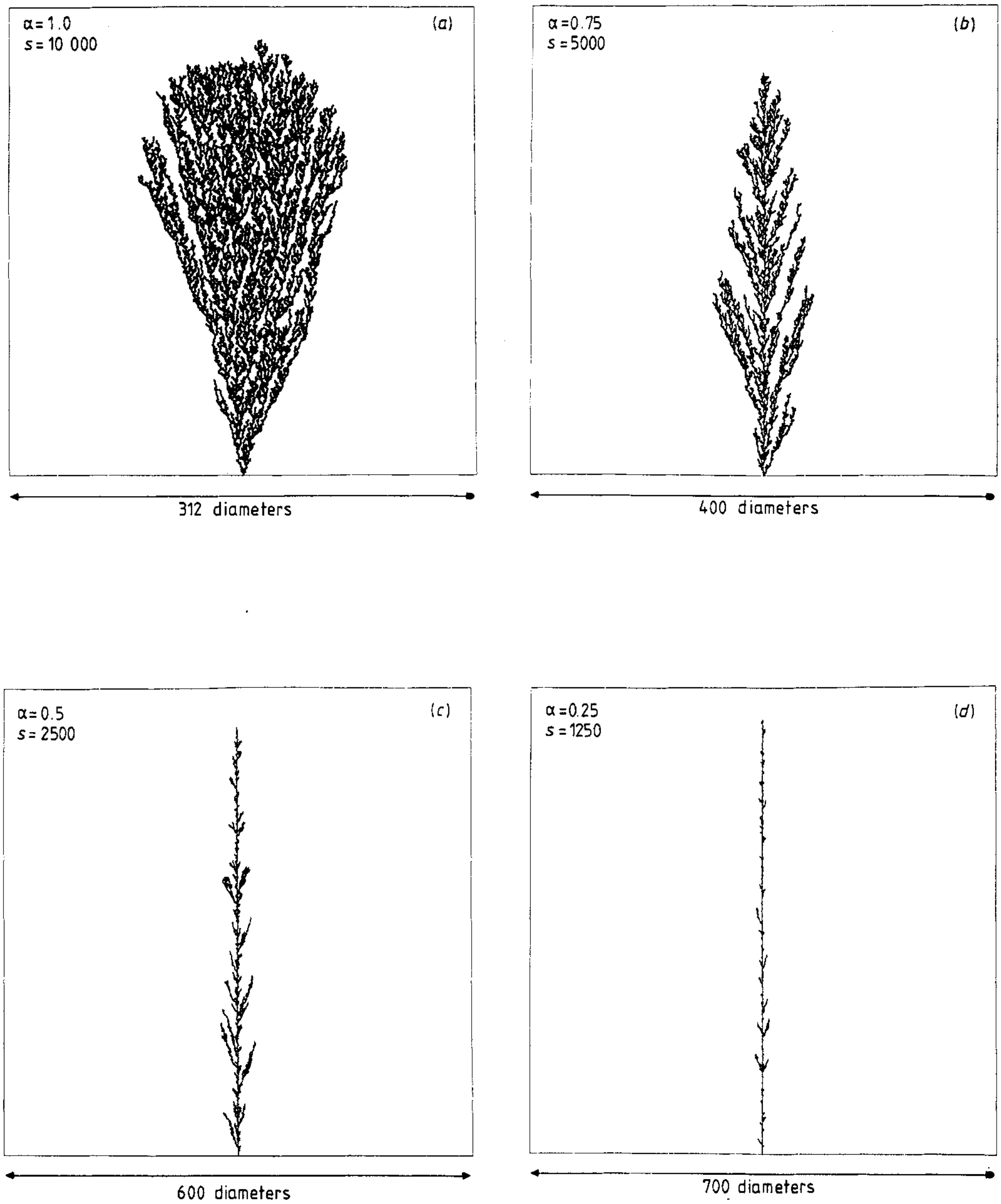


Figure 2. Clusters generated by ballistic aggregation with deposition density distributions given by $\alpha = 1, 0.75, 0.5$ and 0.25 respectively in (a), (b), (c) and (d). (a) ($\alpha = 1$) shows a cluster generated using a uniform deposition density distribution.

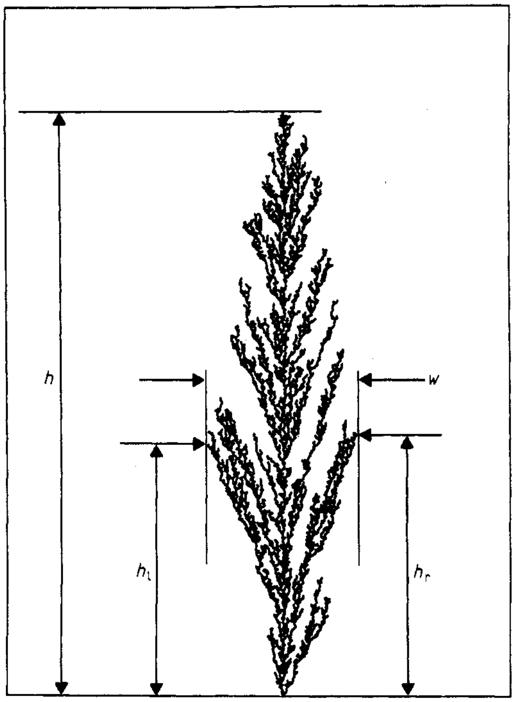


Figure 3. This figure shows the quantities used to partially characterise the shapes of the clusters.

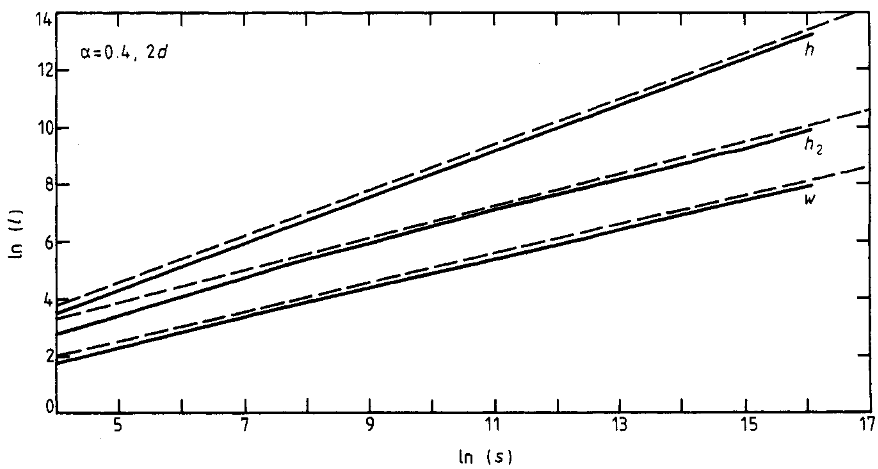


Figure 4. Dependence of the characteristic lengths (l) h, h_2 and w on the cluster sizes obtained from simulations carried out with a singularity strength parameter α of 0.4. The broken lines are straight lines which illustrate the linear dependence of $\ln(l)$ on $\ln(s)$ for all three lengths.

Table 1. Values obtained for the exponents $\nu_\parallel$, $\nu_\perp$ and η from two-dimensional simulations. α is the singularity strength parameter and s is the maximum cluster size (number of particles).

α	s	$\nu_\parallel$	$\nu_\perp$	η
1.0	10^6	0.504	0.501	0.510
0.75	10^6	0.626	0.501	0.501
0.6	10^7	0.701	0.500	0.502
0.5	10^7	0.750	0.500	0.476
0.4	10^7	0.800	0.500	0.549
0.25	10^6	0.875	0.502	0.629
0.125	10^6	0.913	0.501	0.651
0.10	10^7	0.950	0.501	0.714

Similarly, for the case of deposition onto a d_s-dimensional substrate we expect to find that

$$w \sim s^{1(1+d_s)} \sim s^{1/d} \tag{11}$$

and

$$h \sim s^{(d-\alpha)/d}. \tag{12}$$

For the two-dimensional simulations the effective value of the exponent η (equation (6)) has a value close to 0.5 for $\alpha \geqslant 0.5$. For smaller values of α the effective value of η is larger than 0.5 but decreases slowly with increasing cluster size. It seems possible that the asymptotic value for η is 0.5 for all values of $\alpha > 0$.

A similar set of three-dimensional simulations was carried out ($d = 3$, $d_s = 2$) and the results are given in table 2. In this case $\alpha = 2$ corresponds to uniform deposition. The results given in this table are consistent with equation (11) ($\nu_\perp = 1/d$) and (12) ($\nu_\parallel = (d-\alpha)/d$). The effective value for the exponent η remains quite close to $1/d$ for a value of $\alpha \geqslant 1.25$ but for smaller values of α it increases with increasing α.

Based on both the simple arguments given above and the simulation results, the exponents $\nu_\parallel$ and $\nu_\perp$ are given by $\nu_\parallel = (d-\alpha)/d$ and $\nu_\perp = 1/d$. The dependence of η on α is still ambiguous. The computer simulation results indicate that η increases continuously as α decreases and it seems reasonable that η should approach a value of 1 as α decreases. However, this behaviour may be a consequence of a crossover and there may be only two asymptotic values for η.

Table 2. Values obtained for the exponents $\nu_\parallel$, $\nu_\perp$ and η. The statistical uncertainties are about ± 0.0001, ± 0.0002 and ± 0.001 for $\nu_\parallel$, $\nu_\perp$ and η respectively.

α	s	$\nu_\parallel$	$\nu_\perp$	η
2	10^5	0.336	0.345	0.345
1.5	10^6	0.490	0.338	0.331
1.25	2.5×10^6	0.574	0.337	0.363
1.0	2.5×10^6	0.661	0.332	0.430
0.75	2.5×10^6	0.745	0.339	0.509
0.5	10^5	0.833	0.352	0.606
0.25	5×10^6	0.901	0.340	0.705

References

Bensimon P, Shraiman B and Liang S 1984 *Phys. Lett.* **102A** 238
Dirks A G and Leamy H J 1977 *Thin Solid Films* **47** 219
Family F and Vicsek T 1985 *J. Phys. A: Math. Gen.* **18** L75
Henderson D, Brodsky M H and Chaudhari P 1974 *Appl. Phys. Lett.* **25** 641
Kardar M, Parisi G and Zhang Y-C 1986 *Phys. Rev. Lett.* **56** 889
Kim S, Henderson D J and Chaudhari P 1977 *Thin Solid Films* **47** 155
Leamy H J and Dirks A G 1978 *J. Appl. Phys.* **49** 3430
Leamy H J, Gilmer G H and Dirks A G 1980 *Current Topics in Material Science* vol 6, ed E Kaldis, ch 4
Meakin P 1987 *CRC Critical Reviews in Solid State and Materials Science* **13** 143
Meakin P, Ramanlal P, Sander L M and Ball R C 1986 *Phys. Rev.* A **34** 5091
Ottino J M, Leong C W, Rising H and Swanson P D 1988 *Nature* **333** 419
Vold M J 1959a *J. Colloid Sci.* **14** 168
—— 1959b *J. Phys. Chem.* **63** 1608
Witten T A and Sander L M 1981 *Phys. Rev. Lett.* **47** 1400