

# Surface morphology of a modified ballistic deposition model

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The surface and bulk properties of a modified ballistic deposition model are investigated. The deposition rule interpolates between nearest and next-nearest neighbor ballistic deposition and the random deposition models. The stickiness of the depositing particle is controlled by a parameter and the type of inter-particle force. Two such forces are considered - Coulomb and van der Waals type. The interface width shows three distinct growth regions before eventual saturation. The rate of growth depends more strongly on the stickiness parameter than on the type of inter-particle force. However, the porosity of the deposits is strongly influenced by the inter-particle force.

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## I. INTRODUCTION

Surface and structural properties of deposition aggregates are of multidisciplinary interest. Deposition structures occur in various physical, chemical and biological systems and processes. The surface and bulk properties of deposition aggregates are closely related to a wide variety of equivalent problems, such as, fluid flow, adsorption and diffusion in porous structures, directed polymers in random media and propagation of flame fronts [1].

The relation between the geometry and morphology of deposition structures and their formation mechanism has important applications. In recent years, technological advancement and the consequent access to small yet powerful computers have contributed greatly to simulation and numerical studies of deposition structures. Such studies help to develop better understanding and control over the formation of specific forms and surfaces suited to specific purposes. It is of practical relevance in the fabrication of nanomaterials with important applications to industry and medicine, such as, the manufacture of sophisticated optical and electronic nanostructures and nanodevices, magnetic carbon nanostructures for drug delivery [2] and smart nanostructures for monitoring, diagnoses, repair and treatment of human biological systems [3].

Ballistic deposition (BD) is a simple growth model, originally proposed for describing sedimentation and aggregation in colloids [4–7]. This model and its variants give rise to complex porous structures useful for studying formation of sedimentary rock structures and dust agglomerates.

The growing surface is quantitatively expressed in terms of a surface width  $W$ , associated with the rough-

ness of the surface, and is defined as,

$$W(L, t) = \sqrt{\frac{1}{L} \sum_{i=1}^L [h(i, t) - \langle h(t) \rangle]^2} \quad (1)$$

where  $L$  is the system size and  $t$  is the growth time. The surface width obeys a dynamic scaling law [8],

$$W(L, t) \sim L^\alpha f\left(\frac{t}{L^\beta}\right) \quad (2)$$

The exponents  $\alpha$  and  $\beta$  describe the growth of surface width with system size and time.

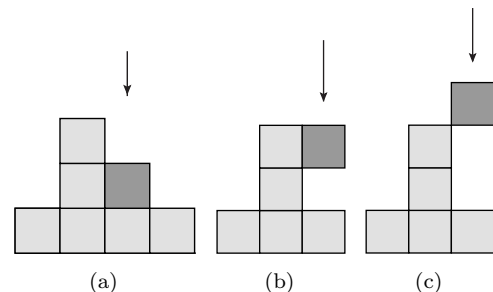


FIG. 1: (a) Random deposition, (b) nearest neighbor (NN) ballistic deposition, (c) next-nearest neighbor (NNN) ballistic deposition

In random deposition (RD), a site on the surface is selected at random. A particle drops vertically and deposits on top of the selected column (Fig. 1a). In nearest neighbor (NN) ballistic deposition, a particle travels in a vertical trajectory towards the randomly chosen site and deposits onto the first surface it encounters. This may be the top of the chosen column or the side of the nearest neighbor column, whichever is higher. In the next-nearest neighbor (NNN) variant of BD, the new particle deposits at the first corner or side or top of column encountered by the particle along its vertical path

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of descent. Fig. 1b and Fig. 1c illustrate the NN and NNN ballistic deposition. In ballistic deposition, the particles are assumed to be strongly adhering and stick to the first point of contact whereas in random deposition, the particle deposits when it cannot go down any further. The roughness of the growing surface grows without bound in RD, while in BD, correlation among neighboring columns, causes the surface roughness to eventually saturate. Unlike random deposition, where the surface growth is only along the upward vertical direction, in the ballistic deposition, the surface grows laterally (for NN) and diagonally (for NNN) as well.

In this work, we investigate the surface properties and bulk structure of a modified BD model where the deposition method interpolates between NN and NNN ballistic and the random deposition (RD) models. The depositing particles are allowed to have varying degrees of stickiness ranging uniformly from rigid, non-sticky to strongly adhering. The role of two types of attractive forces between the adhering particles in the formation of the aggregate is also studied. Depending on the stickiness, the attractive force and the surface profile of the deposit, the incoming particles may stick to the corner or side of the nearest neighbor columns or slide down to deposit on top of the column at the randomly selected site. It is a more realistic model for study of porous deposits formed in nature. The growth of surface roughness with time

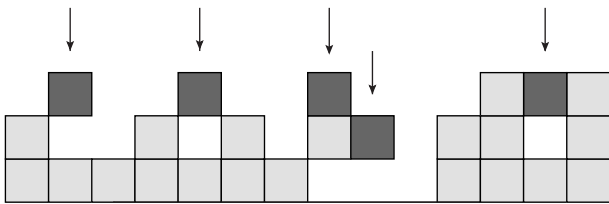


FIG. 2: Possible sticking positions in the present model.

exhibits four distinct regions. The stickiness of the particles is observed to have the most dominant effect on the surface roughness, especially in the intermediate stages of growth of deposit. The surface roughness increases at a far steeper rate than random or KPZ [9] growth. Beyond a certain crossover time, which also varies with the stickiness parameter, the growth of surface roughness slows down to KPZ-like [9] and eventually saturates. Changing the nature of the attractive force between particles from Coulomb to van der Waals, has negligible effect on the behavior of surface width. However, the porosity of the deposit is strongly influenced by the attractive force between particles as well as the stickiness parameter.

## II. FORMULATION OF THE MODEL

In the model discussed in this article, deposition of particles takes place on a one dimensional substrate. Particles drop one by one vertically onto sites selected at random. Two factors contribute to final deposition of

the particle. One is the stickiness of the particle which is varied by means of a parameter denoted by  $a_p$  [10]. The second is an inter-particle attractive force proportional to the center to center distance (denoted here by  $r$ ) between particles. The parameter  $a_p$  is assigned values between 0 and 1, attributing stickiness to the particles. The former value corresponds to no adhesiveness and the latter to maximum stickiness. We have assumed two types of attractive forces, the Coulomb type with an inverse square dependence on  $r$  and the van der Waals type proportional to  $r^{-6}$ . The final sticking position of a newly arriving particle is decided by a sticking probability defined as

$$p_{st} = \frac{a_p}{r^n} \quad (3)$$

where,  $n$  is 2 for Coulomb interaction and 6 for van der Waals interaction. We assume the particles to be unit squares, so that the center-to-center distance is 1 along the side and  $\sqrt{2}$  along the diagonal. A very sticky particle may stick to either the first encountered corner or surface of a neighboring occupied site. A particle which is less sticky, may not stick at the first corner or surface and may slide further down, before final deposition. A new particle may deposit at the top, side or corner of an existing column depending on the sticking probability as illustrated in Fig. 2. Thus, in addition to vertical and lateral growth, the surfaces also grows along an incline of angle  $45^\circ$  or  $135^\circ$  to the horizontal [10].

Simulations are performed starting with an empty substrate for system sizes  $L \simeq 32, 64, 128, 256, 512$  and  $1024$ . A value for the sticking parameter is chosen and for a given type of inter-particle attractive force, the probabilities for corner and side sticking are determined from Eq. 3. Particles are dropped onto randomly chosen sites on the substrate. If the particle falls on a column that is higher than its nearest neighbors, it deposits onto the top of that column. If the neighboring columns are higher, the particle may stick to the corner or side of the tallest neighboring column, provided, the corresponding sticking probability is larger than a random number generated from a uniform distribution between 0 and 1. Else, it slides down vertically till it encounters the next corner or surface, where a similar comparison is made. The process is repeated until deposition occurs.

## III. RESULTS AND DISCUSSION

The numerical simulations were performed for system sizes mentioned above at various values of stickiness parameter ranging from 0.1 to 1.0 in  $(1+1)$  dimension. A logarithmic plot of the interface width versus time at different values of  $a_p$  is shown in Fig. 3. For comparison, the plot for ballistic deposition is also shown in the same figure.

At  $a_p = 0.0$ , the particles deposit onto top of columns randomly. The surface roughness increases without

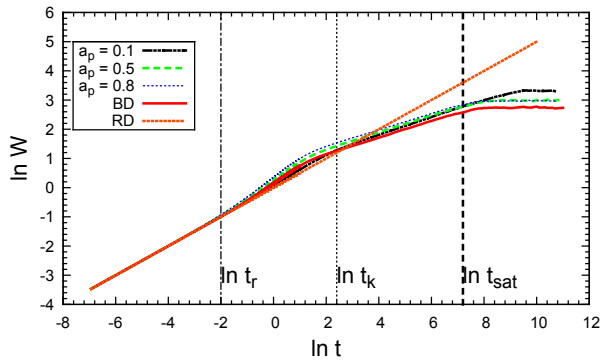


FIG. 3: Logarithmic plot of interface width with time for different  $a_p$ .

bound as more particles deposit. For  $a_p > 0$ , four distinct regions may be identified in the plot. An initial linear region that coincides with RD followed by a step increment of interface width up to a certain time  $t_k$  (see Fig. 3). Thereafter,  $\ln W$  increases, albeit at a much slower rate and eventually, beyond a time  $t_{sat}$ , it saturates. The physical reason for this behavior may be

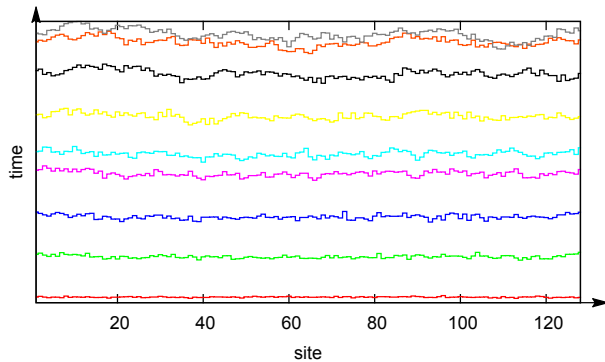


FIG. 4: Evolution of the surface height in the present model

understood as follows. Initially, the deposition process is random as there are few particles and hence for most of the selected sites, there are no neighbors. As more particles get deposited, new arriving particles encounter the corners and sides of those already deposited. The possibility of corner sticking results in the rapid growth of the interface width. The surface roughness thus increases with time as shown in Fig. 4. The deviation of the interface width from random deposition is shown in Fig. 5 for two different values of  $a_p$ . Further deposition slows down the rate of increase of surface roughness. This deviation of the interface width increases with  $a_p$  as the possibility of corner sticking increases. For example, when  $a_p = 0.1$ , the probability for corner sticking is 0.05 and that for side sticking is 0.1, whereas at  $a_p = 0.5$ , the corner sticking probability increases to 0.25 and that for side sticking increases to 0.5. Chances of sticking to corner or side, both increase with  $a_p$ . Hence, the growth along

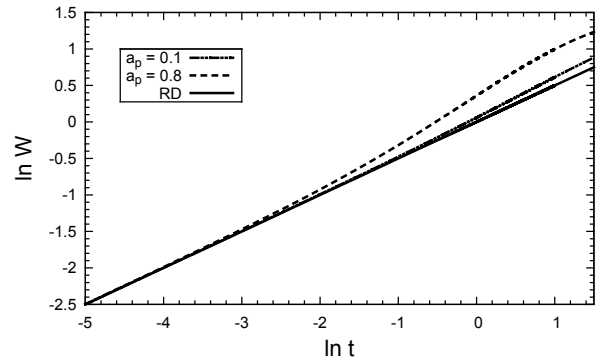


FIG. 5: Deviation from random growth for early times for  $a_p = 0.5$  and  $a_p = 0.8$ .

both lateral and diagonal directions increases with  $a_p$ .

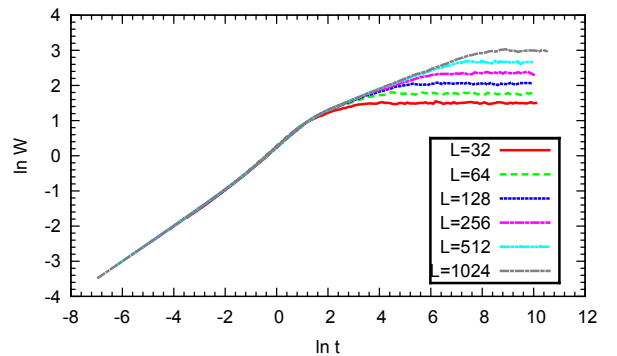


FIG. 6: Variation of interface width with time for different system sizes with  $a_p = 0.5$ .

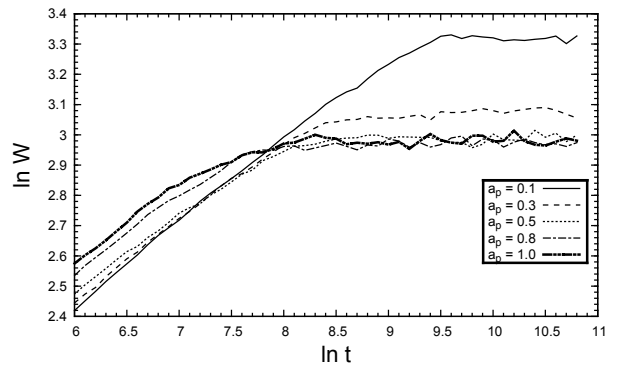


FIG. 7: Variation of interface width with time in the saturated region for  $L = 1024$ .

With further deposition, the increase in surface roughness slows down. Unlike the previous region, this second slower growth region shows a decreasing slope with increase in  $a_p$ . Increase in  $a_p$ , causes more correlations among neighboring columns as the chances of sticking to corner(s) as well as to side(s) increases. As a result, the interface grows at a slower rate.

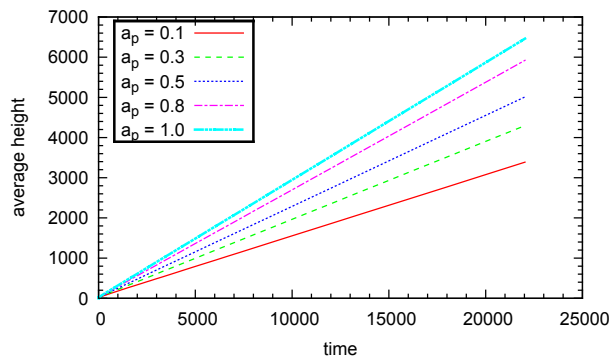


FIG. 8: Evolution of average height at different  $a_p$  for  $L = 256$  and Coulomb type interaction.

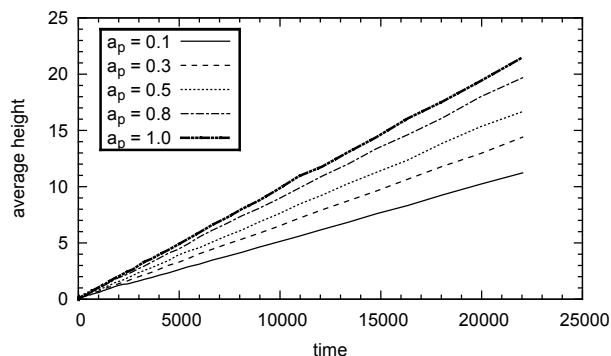


FIG. 9: Evolution of average height at different  $a_p$  for  $L = 256$  and van der Waals type interaction.

Thereafter, with further deposition of particles, the interface width saturates after a time  $t_{sat}$ . The saturated value of the interface width varies with both system size and  $a_p$ . For a given value of  $a_p$ , the saturated width  $W_{sat}$  and the time of saturation,  $t_{sat}$  increase with system size. For a fixed  $a_p$ , the evolution of the interface width for different system sizes is shown in Fig. 6.

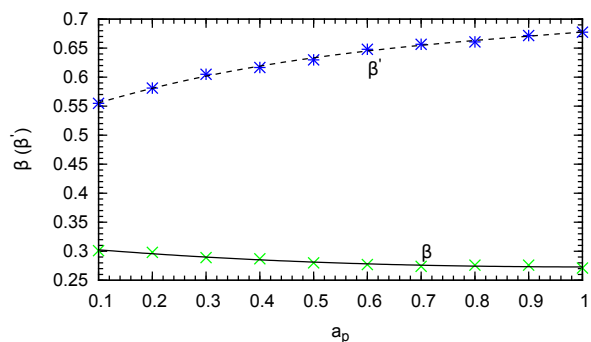


FIG. 10: Variation of  $\beta$  (solid line) and  $\beta'$  (dashed line) with  $a_p$  for  $L = 1024$

With the system size kept fixed, the saturated width

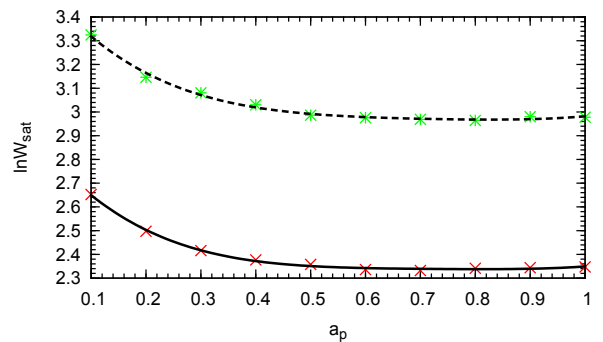


FIG. 11: Saturated width versus  $a_p$  for  $L = 256$  (solid line) and 1024 (dashed line).

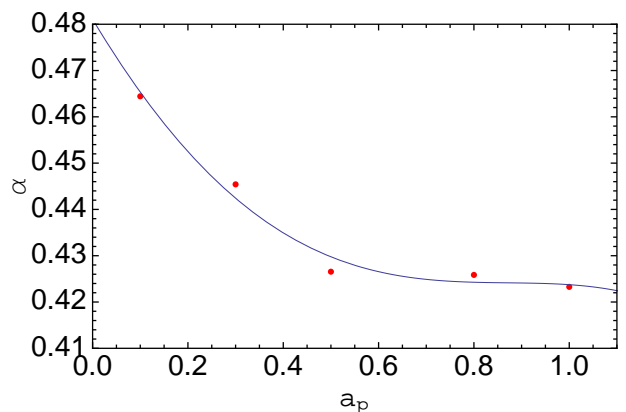


FIG. 12: Variation of  $\alpha$  with  $a_p$

decreases with increase in  $a_p$  and so does the time of saturation. There is a marked decrease in saturated width when  $a_p$  is increased from 0.1 to 0.3. Thereafter, the value of the saturated width shows a very small decrease with further increase in  $a_p$ . This behavior is due to the increase in correlation length as the stickiness parameter increases. However, the correlation length cannot exceed the system size. Hence the decrease in saturated width is most prominent at low values of  $a_p$ . Fig. 7

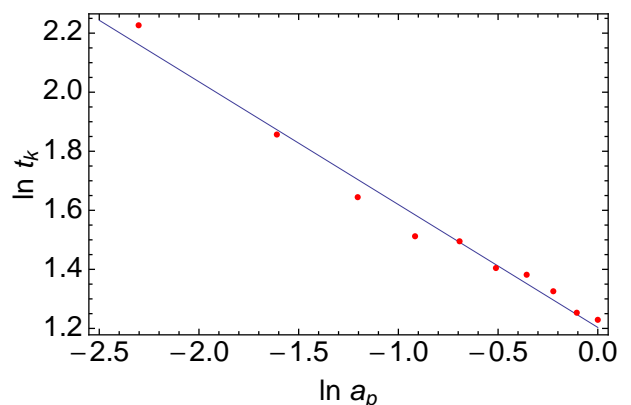


FIG. 13: Logarithmic plot of crossover time  $t_k$  with  $a_p$ .

shows the variation of the saturated interface width  $a_p$  for system size 1024 and Coulomb type interaction. It is also observed that the interface width saturates at earlier time with increase in  $a_p$ . When the inter-particle force is switched to van der Waals type, there is negligible change in growth and the saturation of interface width. Fig. 8 and 9 show the evolution of the average height of the surface for Coulomb and van der Waals type interaction respectively. Though the qualitative nature of the above plots are the same, the average surface height for van der Waals type of interaction is much less than that for Coulomb type interaction. However, for both type of forces, the average height at any time is larger and grows faster for larger values of  $a_p$ .

TABLE I: Values of  $\beta'$  for different  $a_p$

$L$	$a_p = 0.1$	$a_p = 0.3$	$a_p = 0.5$	$a_p = 0.8$	$a_p = 1.0$
128	0.55	0.60	0.63	0.66	0.67
256	0.55	0.60	0.63	0.67	0.67
512	0.55	0.60	0.63	0.66	0.68
1024	0.55	0.60	0.63	0.66	0.68

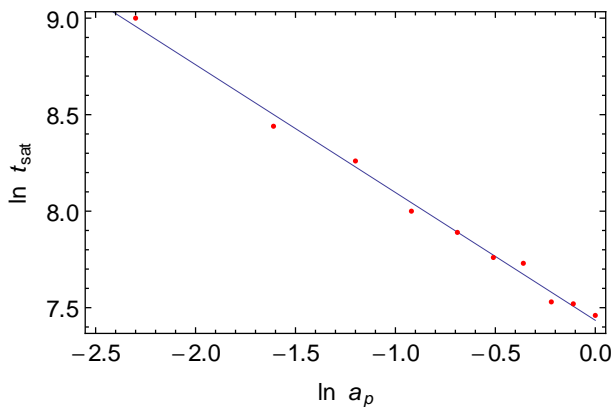


FIG. 14: Saturation time  $t_{sat}$  versus  $a_p$  in log-log scale.

For  $t \ll 1$ , the roughness of interface grows with exponent  $\sim 0.5$  as for random growth. Further deposition causes a sharp increase in the roughness. The values of this growth exponent, denoted by  $\beta'$ , are tabulated below (Table I) for different system sizes and  $a_p$ . For a fixed system size,  $\beta'$  increases with  $a_p$ . However, at any given value of  $a_p$ ,  $\beta'$  does not change with the system size. This behavior is observed for both Coulomb type and van der Waals type attractive forces.

This rapid growth of roughness is not sustained beyond a certain time  $t_k$ . The rate of increase of roughness slows down to a KPZ like growth with a different exponent denoted by  $\beta$ . This exponent, unlike  $\beta'$ , decreases with  $a_p$ . For a fixed  $a_p$ ,  $\beta$  increases with the system size

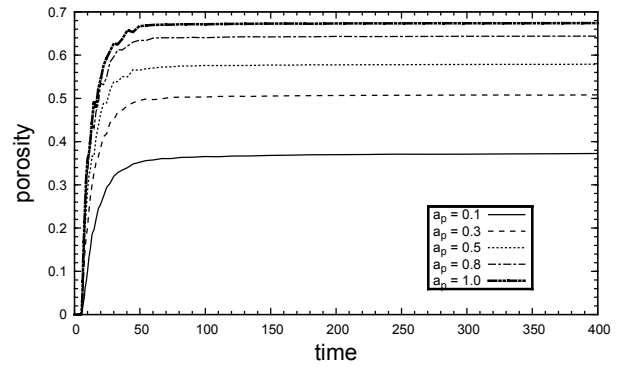


FIG. 15: Growth of porosity at different  $a_p$

approaching a value 0.31. In Table II, values of  $\beta$  (exponent for KPZ like growth) are tabulated for different system sizes and  $a_p$ .

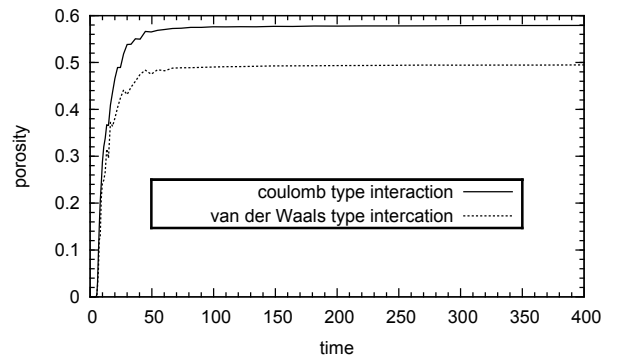


FIG. 16: Growth of porosity for Coulomb and van der Waals type interaction.

In Fig. 10,  $\beta$  and  $\beta'$  are plotted versus  $a_p$  for system size 1024 and a third degree polynomial.

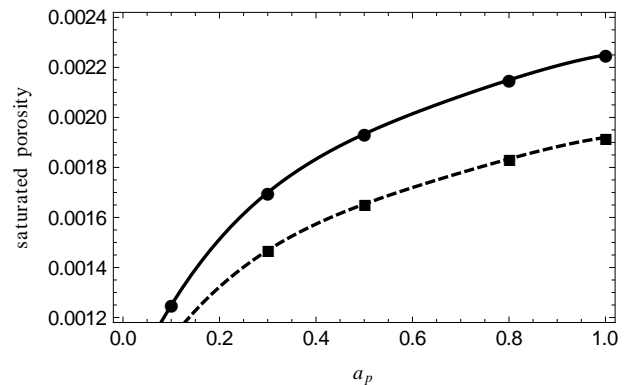


FIG. 17: Saturated Porosity variation with  $a_p$  for Coulomb (solid line) and van der Waals type (dashed line) interaction.

The saturated width at any value of  $a_p$  in the present model is larger than the saturated width in ballistic de-

position. At any value of  $a_p$ , saturated width is larger for larger system sizes as shown in Fig. 11. The saturated width  $W_{sat}$  approaches a limiting value as  $a_p \rightarrow 1$  for a fixed system size. This limiting value is size dependent as shown in Fig. 11.

TABLE II: Values of  $\beta$  for different  $a_p$

$L$	$a_p = 0.1$	$a_p = 0.3$	$a_p = 0.5$	$a_p = 0.8$	$a_p = 1.0$
128	0.2911	0.271721	0.250261	0.24836	0.228566
256	0.289875	0.286438	0.261282	0.25338	0.247328
512	0.29726	0.287251	0.270889	0.265053	0.259155
1024	0.298774	0.297451	0.280052	0.275126	0.270122

Fig. 12 reveals a power law variation of the roughness exponent  $\alpha$  with  $a_p$ . The variation appears to follow a fourth order polynomial.

Corresponding to the four distinct regions, three transition times may be associated. The transition to the rapid growth region from the initial linear RD region is denoted by  $t_r$ . This first transition time, for a given system, is observed to decrease with increase in  $a_p$ . The deviation from RD is due to the fact that the value of the variance determining the roughness of the interface width increases as particles stick more to corners. Increase in  $a_p$  translates into increased possibility of sticking to corners. Hence, the deviation from RD begins sooner. With further deposition of particles, the growth of interface width slows down and shows a KPZ-like growth. The time for this transition is denoted by  $t_k$ .

Fig. 13 shows the power law dependence of crossover time  $t_k$  on  $a_p$ . The logarithmic plot shows  $t_k \sim a_p^{-0.4 \pm 0.04}$  for large system size. The saturated crossover time,  $t_{sat}$ , scales both with the system size  $L$  and  $a_p$  (14). It is observed that,

$$t_{sat} \sim L^z \quad \text{where} \quad z = \frac{\alpha}{\beta} \quad \text{and} \quad t_{sat} \sim a_p^{0.7 \pm 0.03} \quad (4)$$

The  $z$  value obtained by the linear fit of  $t_{sat}$  with system size is  $\sim 1.4$ .

Vacancies or holes in the bulk of the deposit give rise to a porous structure. The porosity may be defined as the fraction of holes (unoccupied sites) in the deposit. For Coulomb type interaction between particles, it is observed that, for any given value of  $a_p$ , the porosity rapidly increases with time and then saturates as shown in Fig. 15. For van der Waals type of interaction, the qualitative nature of the plot is the same. Quantitatively however, the value of porosity is less than that for Coulomb type interaction as shown in Fig. 16. The saturated porosity is found to be independent of the system size. For a fixed system size, it increases with  $a_p$ . The variation of saturated porosity with  $a_p$  for both Coulomb and van der Waals type of interaction is depicted in Fig. 17. The deposit structure formed with van der Waals type of interaction is less porous. A fourth order polynomial gives a good fit to the plot of saturated porosity.

#### IV. CONCLUSION

To summarize, we have studied the bulk and surface properties of deposits formed by particles with varying degrees of stickiness and different inter-particle attractive forces. The stickiness parameter has a more dominant effect on the surface roughness whereas the porosity is rather strongly influenced by the nature of the inter-particle attractive force. In the intermediate stages of growth the surface roughness shows a far steeper rate of increase than in the random or KPZ growth. It would be interesting to derive a continuum stochastic equation corresponding to this growth model and ascertain the role of sticking probability on the coefficient of the various terms of the stochastic equations.

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- [1] F. Family, *Physica A*, **168**, 561 (1990).
  - [2] S. Boncel, A. P. Herman and K. Z. Walczak, *J. Mater. Chem.*, **22**, 31 (2012)
  - [3] K. M. Kummer, E. Taylor, T. J. Webster, *Nanosci. and Nanotechnol. Lett.*, **4**, 483 (2012).
  - [4] M. J. Vold, *J. Colloid Sci.* **14**, 168 (1959); *J. Colloid Sci.* **18**, 684 (1963).
  - [5] D. N. Sutherland, *J. Colloid Interface Sci.* **22**, 300 (1966).
  - [6] F. Family and T. Vicsek, *J. Phys. A* **18**(2), L75 (1985).
  - [7] F. Family, *J. Phys. A* **19**(8), L441 (1986).
  - [8] A. L. Barabasi and H. E. Stanley, *Fractal Concepts in Surface Growth*, Cambridge University Press (1995).
  - [9] M. Kardar, G. Parisi, and Y. C. Zhang, *Phys. Rev. Lett.* **56** (9), 889 (1986).
  - [10] A. Gupta, A. J. Markworth, J. H. Saunder, *J. Mat. Sc* **34**(1999)4141-4147.