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Surface morphology of ballistic deposition with patchy particles and visibility graph

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ABSTRACT

The influence of anisotropic interaction on the morphology of growing clusters formed by patchy particles on 1D substrate has been studied by computer simulations. In this model, the adsorption of the particle occurs only when the 'sticky patch' makes contact with the sticky patch of a previously adsorbed particle. When the patch size p of the particle increases, the morphology of the aggregates changes from the closed structure to a chain like pattern and finally leads to compact thin films. Near the transition, the film is highly porous and the surface roughness $w(t) \sim t$. The structural transition is analyzed by visibility algorithm. The nodes observed near the transition are of high degree. The scale free behavior is observed for all the values of p close to transition with different value of scaling exponents that deviates from expected KPZ behavior.

1. Introduction

Colloidal particles patterned with anisotropic interactions have gained much interest in material science over the past decades. The methods of synthesis are developed and methods such as templating [1], particle lithography [2], nanosphere lithography [3], glance angle deposition [4], capillary fluid flow [5] and colloidal clusters [6] made it possible to prepare particles with 'patches' on their surfaces. These particles interact with each other depending on the size and orientation of the patches unlike colloids that have isotropic interactions. This directionality in the interactions leads to different kinds of the self-assembled exotic structures. The self-assembled structures which are difficult or impossible to observe for the isotropic colloids are now realized with patchy colloids. For example, low coordinated 2D structures [7], helices [8,9] and 3D open lattice structures like diamond [10], empty liquid [11], colloidal gels and glasses [12] are observed. Interestingly, structures which are obtained through the patchy interactions have potential applications in photonics, biomaterials, microelectronics and catalysis [13,14].

The majority of the experimental as wells as theoretical works have been focused on the self-assembling behavior of patchy particles in solution. These studies have been done under equilibrium conditions. But the colloidal particles can also undergo irreversible aggregation, where the force of interaction could be strong and of a short range. The formation of such far from equilibrium structures is studied by a number of kinetic growth models such as the Diffusion Limited Aggregation (DLA) [15], Ballistic Deposition (BD) model [16], Eden model and other variants of these models [17–19]. These models are widely used to understand the formation of structure in various systems like electro-deposition [20–22], crystal growth [23], biological cells [24], viscous fingering [25] and dielectric breakdown [26]. Unlike, the patchy particles interact with each other in a highly anisotropic way which depends on the arrangement and the number of active patches on the surface. A vast number of patchy models has been employed including spot like patchy, rigid body patchy and other extended models with attractive potential in order to understand the structure formation in patchy particle system. The 'Kern–Frenkel potential' has been widely used for simulation of patchy interaction [27]. In this model, when the line joining the centers of the particle intersects with patches on both the particle, it interacts with a square well potential within a range. The growth process critically depends on the angular range of their interaction with other particles. The variable patch range leads to different phases with chain, sheet and compact structures and their behavior is also studied under different external conditions [27–29]. Most of the simulation work explored the variety of the formation of structure and phase behavior in solutions.

Recent focus has been shifted to understand the non-equilibrium properties of patchy colloids with emphasis on growth from substrates. Dias et al. [30] studied the adsorption of patchy colloids on an attractive substrate. They observed three different regions of different densities: surface layer closed to the substrate, a liquid film region with constant density and an interfacial re-

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gion with vanishing density. Another study conducted on colloids with three patches undergoing deposition on a substrate exhibited two absorbing state phase transitions for a lower and a higher value of opening of patch angle [31]. Similarly an absorbing state phase transition is observed by Kartha and Sayeed [32] in patchy colloids undergoing DLA on a 2D interface. Another study was conducted by Dias et al. [33] on the non-equilibrium adsorption of patchy colloids with two types of patches, one at the pole and other at equator to a substrate. The growth process is dominated by two modes of growth; one is chain dominated growth where the density of the film decreases and another is junction dominated growth where film has the constant density. Recently, the interfacial properties of patchy colloids with number of patches, $n > 3$, is studied and shown that the interface is in Kardar–Parisi–Zhang (KPZ) universality class irrespective of anisotropy in bonding interactions [34].

In this paper, we address the non-equilibrium growth of patchy particles from a flat substrate in $(1 + 1)$ dimensions. We have systematically studied the dependence of surface roughness and porosity of the aggregates on the size of the single patch. Considering the previous report on 'Patchy-DLA' studies, where the nature and size of the aggregates was investigated, we have carefully examined the nature of aggregates formed from a one dimensional substrate. This study reports a large disparity in the interface from the expected KPZ class contrary to observation made in [34]. We have also demonstrated the usefulness of the visibility algorithm in understanding the morphological transition in film with anisotropic interaction for the first time.

In the following section we describe the model used in the present study. In sec. 3, we quantify the result by illustrating the nature of the clusters and exhibit the kinetics of surface features of growth process of the non-equilibrium adsorbed film. The porosity of the aggregates is also presented in this section. Finally, in sec. 4, we draw some conclusions.

2. Model description

In the present study, we consider patchy particles with attractive patches on their surfaces. The anisotropic interaction is introduced by a variant form of 'Kern–Frenkel model' proposed for studying aggregation of the colloidal particles with anisotropic interaction [27–29]. The model of particle and patchy–patchy interactions are described in Fig. 1. In this model, a two dimensional particle is a circular disc with two parts. One of them is a patchy part with semi angular range of interaction α and other is a non-sticky part (Fig. 1(a)). The patch size is represented by a parameter $p = \alpha/\pi$ which is proportional to the area of the patch and in the range [0 to 1]. The orientation of the patch is described by a vector v, which bisects the sticky patch and is uniformly distributed. An irreversible bond exists between the neighboring particles if the line connecting the centers of two particles passes through sticky patches of both particles (Fig. 1(b)), otherwise the bonding fails as shown in Fig. 1(c) and Fig. 1(d).

In the standard BD model, the particles are launched from random positions into the substrate while they are normal to the substrate. The particles irreversibly attaches into the first point of contact. Therefore BD growth creates overhangs and voids in the structure. In the present study, we have considered a modified BD growth model. In this model, a particle is randomly selected on a column with random orientation v from uniform distribution of angles in the interval $[0, 2\pi])$. The growth rules of the present study are as follows:

i) The particle is adsorbed to the substrate irrespective of the orientation.

ii) The particle is adsorbed, if the adsorbing condition is met (see Fig. 1(b)).

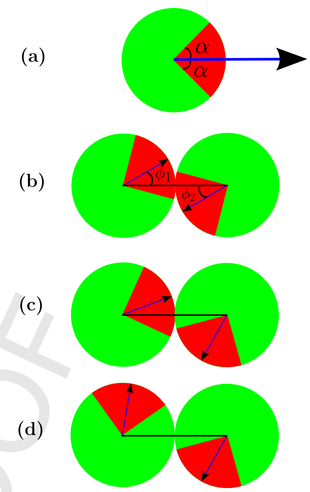

Fig. 1. (Color online.) **(a)** Schematic representation of patchy particle with single patch (red arc) with orientation specified by the vector **v**, and the limits of angular interaction is specified by the angle α. **(b)** Particle adsorption condition. **(c)** and **(d)** non-adsorbing condition.

iii) If this condition is not met (see Fig. 1(c) or (d)), it descends in the same column and searching all sites to find a position having the required condition. If not, then it is removed.

In the present study, the original BD model is regained for $p = 1.0$. Simulations are performed on an empty lattice for the size $L = 1280$. Periodic boundary conditions are applied along the horizontal direction. The number of L particle launches provides the measure of time. All the simulation results were obtained for time $t = 10^4$ which includes approximately 10^7 particle launches. The patch size p is varied from 0.1 to 1.0 in the present study. All the quantities are averaged over 100 independent realizations.

3. Results and discussions

3.1. Surface morphology of aggregates

The numerical simulations were performed for the above mentioned lattice size at various values of patch size p in $1 + 1$ dimensions. We have investigated the effect of the patch size on the morphology of films.

Fig. 2 gives the typical structure of the clusters for different values of p. It is clear from this figure that when the patch size is small, $p < 0.6$, the film grows only for few layers. The physical reason for this growth behavior may be understood as follows; Initially the particles randomly deposited into the substrate. When the patch size is small, new arriving particle finds a 'dead site' and the growth eventually stops. In Fig. 2(a), the dead-end of the already deposited particle is clearly visible. In Ref. [32], a DLA model with patchy particles was introduced. When the patch size is small, $p < 0.6$, an 'absorbing state' with the clusters of small sizes ranging 10–15 particles is observed. Similar to our observations, another study on the growth of particles with three patches on their surface [35] reported a suppressed growth of patchy particle cluster when all the patches lie in same hemisphere.

Fig. 3(b–c) shows the snapshots of the system for $p = 0.6454$, $p = 0.67$ and $p = 0.8$ respectively. When the patch size is $0.6 < p < 0.8$, a ramified network of cluster growth is observed. The nature of the cluster indicates that roughness of the interface depends on p in this region. We have observed long tree like features for $p \sim 0.645$ leading to a 'growing phase', when the patch size was further increased and finally, the structure evolves towards the normal BD compact structure (Fig. 3(c)). The surface pinning effects at certain sites due to capping accompanied by the anisotropy

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