Irreversible Deposition on a Triangular Lattice

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Abstract. Random sequential adsorption of binary mixtures of extended objects on a two-dimensional triangular lattice is studied numerically by means of Monte Carlo simulations. The depositing objects are formed by self-avoiding random walks on the lattice. We concentrate here on the influence of the symmetry properties of the shapes on the kinetics of the deposition processes in two-component mixtures. Approach to the jamming limit in the case of mixtures is found to be exponential, of the form: $\theta(t) \sim \theta_{jam} - \Delta\theta \exp(-t/\sigma)$, and the values of the parameter σ are determined by the order of symmetry of the less symmetric object in the mixture. Depending on the local geometry of the objects making the mixture, jamming coverage of a mixture can be either greater than both single-component coverages or it can be in between these values. Results of the simulations for various fractional concentrations of the objects in the mixture are also presented.

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Random sequential adsorption (RSA) has attracted a considerable interest due to its importance in many physical, chemical, and biological processes. In two dimensions (2D), RSA is a typical model for irreversible and sequential deposition of macromolecules at solid/liquid interfaces. Some examples of the wide range of applicability of this model include adhesion of colloidal particles, as well as adsorption of proteins to solid surfaces, with relaxation times much longer than the formation time of the deposit. A comprehensive survey on RSA is given by Evans [1].

The simplest RSA model is defined by the following three rules: (i) objects are placed one after another in random position on the substrate; (ii) adsorbed objects do not overlap; and (iii) adsorbed objects are permanently fixed at their spatial positions (neither diffusion nor desorption from the surface are allowed). When the surface is saturated by adsorbed objects so that no further objects can be placed, the system reaches the jamming limit. A quantity of central interest is the coverage $\theta(t)$, which is the fraction of the total substrate area occupied by the adsorbed objects at time t. Asymptotic approach of the coverage fraction $\theta(t)$ to its jamming limit $\theta_{jam} = \theta(t \to \infty)$ is known to be given by an algebraic time dependence for continuum systems [2], and by exponential time dependence for lattice models [3]:

$$\theta(t) \sim \theta_{jam} - \Delta\theta \exp(-t/\sigma), \quad (1)$$

where $\Delta\theta$ and σ are parameters that depend on the shape and orientational freedom of depositing objects [3].

In this paper we study the irreversible deposition of two-component mixtures of extended objects on a 2D triangular lattice by Monte Carlo simulations. Here we focus our interest on the influence of the order of symmetry axis of the shape on the kinetics of the deposition processes in two-component mixtures.

DEFINITION OF THE MODEL AND THE SIMULATION METHOD

Simulations are performed for objects of various shapes. The depositing shapes are modeled by directed self-avoiding walks on 2D triangular lattice. A self-avoiding shape of length ℓ is a sequence of *distinct* vertices $(\omega_0, \ldots, \omega_\ell)$ such that each vertex is a nearest neighbor of its predecessor, i.e., a walk of length ℓ covers $\ell+1$ lattice sites. Examples of such walks for various lengths ℓ are shown in Table 1. On a triangular lattice objects with a symmetry axis of first, second, third, and sixth order can be formed.

At each Monte Carlo step a lattice site is selected at random. If the selected site is unoccupied, one of the six possible orientations is chosen at random and deposition of the object is tried in that direction. We fix the beginning of the walk that makes the shape at the selected site and search whether all successive ℓ sites are unoccupied. If so, we occupy these $\ell+1$ sites and place the object. If the attempt fails, a new site is selected, and so on. After long enough time a jamming limit is reached when there is no more possibility for a deposition event. In the case of mixtures, at each Monte Carlo step a lattice site and one of the objects that make the mixtures are selected at random.

The Monte Carlo simulations are performed on a triangular lattice of size $L = 120$. Periodic boundary conditions are used in all directions. The time is counted by the number of attempts to select a lattice site and scaled by the total number of lattice sites. The data are averaged over 500 independent runs for each shape and each mixture of shapes.

RESULTS AND DISCUSSION

For all the objects from Table 1 and for all the mixtures from Table 2 plots of $\ln(\theta_{jam} - \theta(t))$ vs t are straight lines for the late stages of deposition. These results are in agreement with the exponential approach to the jamming limit of the form (1), with parameters σ, A and θ_{jam} that depend on the shape of the depositing object, i.e. on the combination of the objects making the mixture. The values of the parameter σ are determined from the slopes of the lines and they are given in Table 1. According to σ, all shapes can be divided into four groups: shapes with a symmetry axis of first order with $\sigma \simeq 5.9$; shapes with a symmetry axis of second order with $\sigma \simeq 3.0$; shapes with a symmetry axis of third order with $\sigma \simeq 2.0$; shapes with a symmetry axis of sixth order with $\sigma \simeq 0.99$. This means that the rapidity of the approach to the jamming limit depends on the order of symmetry of the shape and the approach is slower for less symmetric shapes.

In the case of mixtures the value of the parameter σ is determined by the order of symmetry of the less symmetric object in the mixture and the values are: $\sigma \simeq 11.6$ for the mixtures including an object with a symmetry axis of first order; $\sigma \simeq 5.65$ for the mixtures that contain at least one object with symmetry axis of second order and no objects with symmetry axis of first order; $\sigma \simeq 3.97$ for the mixtures that contain at least

TABLE 1. Parameters $\Delta\theta$ and σ for various shapes. The typical statistical errors are estimated to the last given digits.

(x)	shape	$n_s^{(x)}$	$\ell^{(x)}$	$\theta_{jam}^{(x)}$	$\Delta\theta$	σ
(A)		2	1	0.9139	0.105	3.12
(B)		2		0.8362	0.134	2.94
(C)		1	2	0.8345	0.0813	5.78
(D)		3		0.7970	0.115	1.96
(E)		2		0.7212	0.0954	2.84
(F)		6	6	0.6695	0.0773	0.994
(G)		1		0.6443	0.0721	6.07

TABLE 2. Coverage fraction $\theta_{jam}^{(x)+(y)}$ for various binary mixtures. The typical statistical errors are estimated to the last given digits.

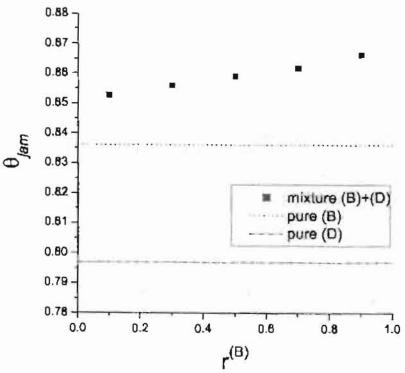
$(x)+(y)$	shapes	$n_s^{(x)}+n_s^{(y)}$	$\theta_{jam}^{(x)+(y)}$	$\Delta\theta$	σ
$(A)+(B)$	+	2 + 2	0.9202	0.125	5.52
$(B)+(C)$	+	2 + 1	0.8526	0.0365	11.42
$(B)+(D)$	+	2 + 3	0.8591	0.0781	5.51
$(C)+(D)$	+	1 + 3	0.8624	0.0493	11.62
$(E)+(F)$	+	2 + 6	0.7125	0.0344	5.76
$(E)+(G)$	+	2 + 1	0.6833	0.0437	11.22
$(F)+(G)$	+	6 + 1	0.7087	0.0450	11.57

one object with symmetry axis of third order and no objects with symmetry axis of lower order; $\sigma \simeq 0.985$ for the mixtures of the objects with symmetry axis of sixth order [4].

In the late stages of deposition the less symmetric objects have to try all possible orientations, so they are responsible for the approach to the jamming limit. Deposition of mixtures is slower in comparison to the deposition of pure objects, except for the objects with symmetry axis of sixth order for which the parameter σ has the same values for the pure shapes and for the mixture.

Value of θ_{jam} for a mixture depends on the local geometry of the objects making the mixture. Comparing the results from Table 1 and Table 2 we can see that for a number of combinations of depositing objects the jamming coverage for a mixture has greater values than the jamming coverages for the pure shapes making the mixture. However, there are also mixtures such as $(E)+(F)$, $(E)+(G)$ that have a lower jamming coverage than one of the components. The jamming coverage of the mixtures is still greater than the jamming coverage of the other component. The mutual feature of these mixtures is that the jamming coverages of their components differ significantly.

We have also performed extensive simulations in order to investigate the deposition processes for various fractional concentrations $r^{(x)}$ and $r^{(y)}$ of the shapes (x) and (y) in the reservoir, i.e. for various probabilities for choosing one of these shapes for a deposition attempt. In Fig. 1 jamming coverages obtained for various compositions of mixtures $(x)+(y)$ are shown vs the fractional concentration $r^{(x)}$ $(r^{(y)} = 1 - r^{(x)})$. We



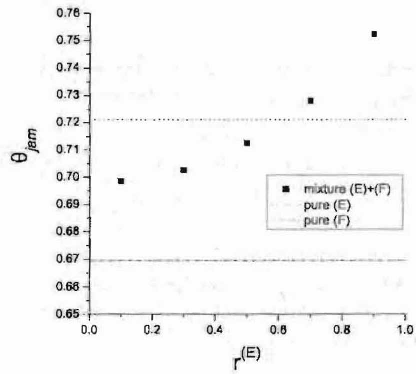


FIGURE 1. Jamming coverages for the mixtures vs the fractional concentration

can see that θ_{jam} varies monotonously with the fractional concentration of one of the objects, growing with the concentration of the object with greater jamming coverage of the pure shapes. Depending on the combination of the objects and on their fractional concentrations it can be either greater than both jamming coverages of the pure shapes making the mixture or it can be lower than the higher single-component jamming coverage, but still higher than the other.

CONCLUDING REMARKS

Kinetics of irreversible deposition of mixtures on a triangular lattice has been studied by Monte Carlo simulations. The approach to the jamming limit was found to be exponential for all the shapes and all the mixtures. The rapidity of the approach depends only on the symmetry properties of depositing objects. For two-component mixtures the value of the parameter σ is determined by the order of symmetry of the less symmetric object in the mixture.

Jamming coverage for a mixture is always greater than the jamming coverage of the component with lower θ_{jam} and it is often greater than either of the jamming coverages of the components making the mixture.

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