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Response properties in the adsorption–desorption model on a triangular lattice

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HIGHLIGHTS

- Reversible RSA of objects of various shapes on a 2D triangular lattice is studied.
- We study the response of the model to an abrupt change in desorption probability.
- Short-time response strongly depends on the symmetry properties of the shapes.
- Density correlations decay slower for more symmetrical shapes.
- We observe the weakening of correlation features in multicomponent systems.

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ABSTRACT

The out-of-equilibrium dynamical processes during the reversible random sequential adsorption (RSA) of objects of various shapes on a two-dimensional triangular lattice are studied numerically by means of Monte Carlo simulations. We focused on the influence of the order of symmetry axis of the shape on the response of the reversible RSA model to sudden perturbations of the desorption probability P_d. We provide a detailed discussion of the significance of collective events for governing the time coverage behavior of shapes with different rotational symmetries. We calculate the two-time density–density correlation function $C(t, t_w)$ for various waiting times t_w and show that longer memory of the initial state persists for the more symmetrical shapes. Our model displays nonequilibrium dynamical effects such as aging. We find that the correlation function $C(t, t_w)$ for all objects scales as a function of single variable $\ln(t_w)/\ln(t)$. We also study the short-term memory effects in two-component mixtures of extended objects and give a detailed analysis of the contribution to the densification kinetics coming from each mixture component. We observe the weakening of correlation features for the deposition processes in multicomponent systems.

1. Introduction

The understanding of random sequential adsorption (RSA) model has attracted large attention as a paradigmatic approach towards irreversibility, as well as due to the strong departure of the process from equilibrium behavior. In the RSA model [1], particles are added randomly and sequentially onto a substrate without overlapping each other. RSA model assumes that

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deposited particles can neither diffuse along, nor desorb from the surface. The kinetic properties of a deposition process are described by the time evolution of the coverage $\theta(t)$, which is the fraction of the substrate area covered by the adsorbed particles. Within a monolayer deposit, each adsorbed particle affects the geometry of all later placements. Due to the blocking of the substrate area, at large times the coverage approaches the jammed-state value θ_J, where only gaps too small to fit new particles are left in the monolayer.

In pursuit of understanding the various aspects of the adsorption phenomenon large number of studies have taken place. A comprehensive survey on RSA and cooperative sequential adsorptions is given by Evans [2]. Other surveys include Privman [3–5], Cadilhe et al. [4], Senger et al. [6], and Talbot et al. [7].

In many real physical situations it is necessary to consider the possibility of desorption of deposited particles [8–10]. Adsorption–desorption processes are important in the binding of ions to a Langmuir monolayer [11], and in many catalytic reactions. Binding and unbinding of kinesin motors to microtubules [12], of myosin to actin filaments, and of proteins to DNA are commonly studied biological examples. Possibility of desorption makes the process reversible and the system ultimately reaches an equilibrium state when the rate of desorption events balances the rate of adsorption events. The kinetics of the reversible RSA is governed by the ratio of adsorption to desorption rate, $K = k_+/k_-$. For large values of K, there is a rapid approach to density $\theta \simeq \theta_J$, followed by a slow relaxation to a higher steady-state value θ_∞ [13–16].

The reversible RSA model is frequently used by many authors to reproduce qualitatively the densification kinetics and other features of weakly vibrated granular materials [9,17,10]. The phenomenon of granular compaction involves the increase of the density of a granular medium subjected to shaking or tapping [18–23]. The relaxation dynamics is extremely slow, taking many thousands of taps to approach the steady state, and it slows down for lower vibration intensities. The final steady-state density is a decreasing function of the vibration intensity [23]. Dynamics of the reversible RSA model depends on the excluded volume and geometrical frustration, just as in the case of granular compaction. This model can be regarded as a simple picture of a horizontal layer of a granular material, perpendicular to the tapping force. As a result of a tapping event, particles leave the layer at random and compaction proceeds when particles fall back into the layer under the influence of gravity. The ratio of desorption to adsorption rate $1/K = k_-/k_+$ within the model plays a role similar to the vibration intensity Γ in real experiments [24] (Γ is defined as the ratio of the peak acceleration of the tap to the gravitational acceleration g).

One of the striking features of granular materials are the memory effects observed by measuring the short-time response to an instantaneous change in the tapping acceleration Γ [25]. For a sudden decrease in Γ it was observed that on short-time scales the compaction rate increases, while for a sudden increase in Γ the system dilates for short times. This behavior is transient and after several taps there is a crossover to the "normal" behavior, with the relaxation rate becoming the same as in constant vibration intensity mode. Furthermore, Nicolas et al. [26] have also shown that periodic shear compaction exhibits a nontrivial response to a sudden change in shear amplitude. The rapid variation of volume fraction induced by the sudden change of shear angle is proportional and opposite to the angle change. The short-term memory effects observed in granular materials are reflected in the fact that the future evolution of the packing fraction θ after time t_w depends not only on the $\theta(t_w)$, but also on the previous tapping history. It is important to note that the parking lot model (PLM, 1D off-lattice reversible RSA model) [24,9,27,17] is a widely used model which can reproduce qualitatively the short-term memory effects of a weakly vibrated granular material. In Ref. [10] we have presented the detailed studies of the short-term memory effects in the framework of a two-dimensional reversible RSA model on a square lattice.

An important issue in two-dimensional deposition is the influence of the shape of the adsorbed particle. It is well known that the size, aspect ratio and symmetry properties of the object have a significant role in the processes of both irreversible and reversible deposition. The numerical analyses for the irreversible deposition of various shapes and their mixtures on a triangular lattice [28,29] establish that the approach to the jamming limit follows the exponential law with the rate dependent mostly on the order of symmetry axis of the shape. In the reversible case of deposition on a triangular lattice [15,30], we have found that the coverage kinetics is severely slowed down with the increase of the order of symmetry of the shape.

The main goal of the present study is to investigate the interplay between the response of the reversible RSA model to sudden perturbations of the desorption probability P_d and the symmetry properties of deposited shapes. Numerical simulations of adsorption–desorption processes are performed for various shapes on the triangular lattice, shown in Table 1. These shapes are made of self-avoiding walks of the same length $\ell = 2$, but they differ in their symmetry properties. The response in the evolution of the density $\theta(t)$ to a change in the desorption probability P_d at a given time t_w is accompanied by transformation of the local configurations in the covering. Essentially, collective (two-particle) events are responsible for the evolution of θ for $\theta > \theta_J$. Size of the objects and their symmetry properties have a significant influence on these collective events, thus affecting the kinetics of the deposition process [15,31,30]. Since we focus our interest on the influence of symmetry of the object on the response of the system to sudden perturbation of the desorption probability P_d, it is necessary to analyze the processes with the objects of the same size. In this paper we also study the response of two-component mixtures of extended objects (see, Table 1) to sudden perturbations of the desorption probability P_d. We did carry out a detailed analysis of the contribution to the densification kinetics coming from each mixture component. Finally, we study the nonequilibrium two-time density–density correlation function $C(t, t_w)$. We focus, in particular, on the influence of symmetry properties of the shapes on the decay of $C(t, t_w)$ and aging effects. This work provides for the first time the link between the short-term memory effects and intrinsic properties of the shapes.

Recently, we have analyzed the growth of the coverage $\theta(t)$ above the jamming limit to its steady-state value θ_∞ within the framework of the adsorption–desorption model of dimers in one dimension [32]. We reported a numerical evidence