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PERCOLATION ON A TRIANGULAR LATTICE UNDER ANISOTROPIC CONDITIONS

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Abstract. The properties of percolation of objects of various shapes on a two-dimensional triangular lattice is studied by means of Monte Carlo simulations. Depositing objects of various shapes and sizes are made by directed self-avoiding walks on the lattice. Anisotropy is introduced by positing unequal probabilities for orientation of depositing objects along different directions of the lattice. This probability is equal p or $(1-p)/2$, depending on whether the randomly chosen orientation is horizontal or not, respectively. It is found that the percolation threshold θ_p increases with the degree of anisotropy, having the maximum values for fully oriented objects.

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1. Introduction

Random sequential adsorption of extended objects at different surfaces is of considerable interest for a wide range of applications in biology, nanotechnology, device physics, physical chemistry, and materials science [1]. In the RSA model objects of a specified shape are randomly and sequentially deposited onto a substrate without overlapping each other. The adsorbed particles are permanently fixed at their spatial positions and they affect the geometry of all later placements so the jamming coverage θ_{jam} is less than in close packing. 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 occupied by the adsorbed particles. For discrete substrates the late time kinetics of the process is described by the time dependence:

$$\theta(t) = \theta_{jam} - Ae^{-t/\tau}, \tag{1}$$

where A and τ are parameters that depend on the shape, orientational freedom of the objects, and on the substrate dimensionality and heterogeneity.

During the process of irreversible deposition, coverage increases causing the growth of clusters of occupied sites. Percolation assumes the formation

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of a large cluster that connects two opposite sides of the substrate [2]. In order to describe the inhomogenuous surfaces in the RSA model, anisotropy in the deposition procedure can be imposed [3]. Namely, the probability for deposition is different along different directions of the underlying lattice. This simple modification introduces preferential direction in the deposition process and causes a specific "patterning" of the deposited layer.

The aim of this research was to investigate the percolation properties in irreversible deposition of objects of various shapes under anisotropic conditions, with various probabilities p for depositions in a certain direction, i.e. for various values of the order parameter.

2. Definition of the model and the simulation method

Anisotropic irreversible deposition of extended objects that are modeled by self-avoiding walks on a triangular lattice (Table I) is studied by Monte Carlo simulations. Simulations are performed for k-mers (denoted as (A), angled objects (B), and triangles (C) up to the length $\ell = 20$, and for rhombuses (D) less then $\ell = 15$ because the percolation cannot be reached for larger ones.

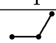
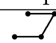
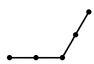
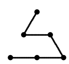
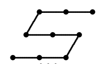
shape	$A\ell$	shape	$B\ell$	shape	$C\ell$	shape	$D\ell$
	$\ell = 1$		$\ell = 2$		$\ell = 2$		$\ell = 3$
	$\ell = 2$		$\ell = 3$		$\ell = 5$		$\ell = 8$
...	...	...	...	...	...	...	...
...	$\ell = 10$	...	$\ell = 20$	...	$\ell = 20$	...	$\ell = 24$

TABLE I: Illustration of the construction of objects larger than basic ones. Simulation are performed for line segments (k-mers) Al; angled objects of sizes Bl; triangles Cl and rhombuses Dl.

Anisotropy is introduced by imposing different probabilities of deposition in the three possible directions. The choice of the horizontal direction occurs with probability p and for each of the other two directions with probability $(1 - p)/2$. Hence, the value of $p = 1/3$ corresponds to the isotropic case. The probability p actually stands for the order parameter characterizing the degree of anisotropy.

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 with the corresponding probability and deposition of the object is tried in that orientation. 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 at random. The jamming limit is reached when the object of the specified shape can't be placed in any position on the lattice. The coverage of the surface is increased in the RSA process up to the percolation threshold, when there appears a cluster that extends through the whole system - from the left to the right side of the lattice. The tree-based union/find algorithm is used to determine the percolation threshold [4].

The Monte Carlo simulations are performed on a triangular lattice of size up to $L = 3200$. 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. In all the simulations the data are averaged over 500 independent runs.

3. Results and discussion

Jamming coverages and percolation thresholds are determined for a large variety of objects shown in Table I. The effective percolation threshold θ_p, measured for a finite lattice, approaches the asymptotic value θ_p^* $(L \to \infty)$ via the power law:

$$\theta_p - \theta_p^* \propto L^{-1/\nu} \; . \tag{2}$$

The theoretical value for the critical exponent is $\nu = 4/3$ for two-dimensional systems. The validity of the finite-size scaling is confirmed in the whole range of parameter p. Moreover, the asymptotic value of the percolation threshold θ_p^* coincides with the value of θ_p obtained for the largest lattice, within the limits of the statistical error. Scaling of the standard deviation σ_p, according to the relation:

$$\sigma_p \propto L^{-1/\nu} \; , \tag{3}$$

was plotted in a way that the values of σ_p are shown vs. L on a log-log scale and they lie on parallel straight lines. The slope of these lines corresponds to the exponent $1/\nu = 0.75 \pm 0.01$, so the results of simulations confirmed the theoretical value of critical exponent.

Results for jamming densities and percolation thresholds are obtained for various values of the order parameter p ranging from $p = 0$ to $p = 1$. Dependence of the percolation threshold θ_p on the order parameter p are presented in Figure 1 for various sizes of the basic objects from Table I. It can be seen that the lowest values of θ_p are obtained for the isotropic case ($p = 1/3$). Percolation threshold increases with the degree of anisotropy, having the largest values for fully oriented objects in one direction ($p = 1$). This property is most pronounced for k-mers (Fig. 1 a)). On the other hand, for triangles (C), neither jamming nor percolation are affected by the anisotropy (Fig. 1 c)). The relative increase of the percolation threshold due to the complete alighnement (maximum anisotropy) defined as:

$$R = \frac{\theta_p(p = 1) - \theta_p(p = 1/3)}{\theta_p(p = 1/3)} \; , \tag{4}$$

is largest for the k-mers of length $\ell = 11$ ($A11$), and its value is 28.6%. Simulations has shown that the impact of anisotropy on the percolation properties is largest for the elongated objects (A) on the contrary to the compact rhombuses (D), that are less affected by the anisotropic conditions. With the exception of fully symmetrical objects, the increase in the anisotropy always results in higher percolation thresholds. It should be emphasized that the statistical errors are typically of the order of 10^{-3}, and in all the figures the error bars are smaller than the symbol size.

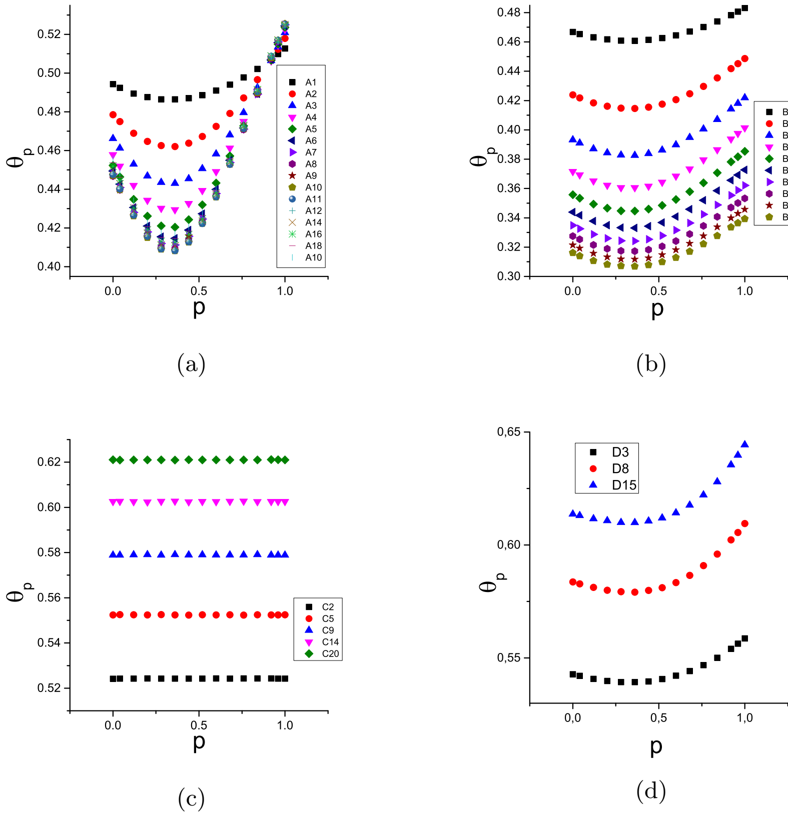


FIG. 1: Dependence of the percolation threshold θ_p on the probability p for deposition in the horizontal direction, i.e. on the order parameter, for various basic objects from Table I and for the larger sizes of these shapes: a) (A); b) (B); c) (C); d) (D)

In the isotropic case, percolation threshold decreases with ℓ for shorter k-mers, reaches a smooth minimum for $\ell \simeq 11$, and slightly increases for longer k-mers [5]. Dependence of the percolation threshold on the length of various objects from Table I is shown in Figure 2 for the values of the order parameter: $p = 0$; 0.12; 0.28; 0.44; 0.60; 0.76; 0.92 and 1. Introducing the anisotropy shifts the minimum towards lower k-mer lengths. For highly anisotropic conditions a qualitatively different behavior is obtained - θ_p increases with the k-mer length, reaches a maximum, and decreases for longer k-mers (Fig. 2 a)). For the angled objects (B) θ_p decreases with ℓ (Fig. 2 b)), but for the triangles (C) increases with the object size (Fig. 2 c)). There is an essential difference between deposition of elongated objects and the compact ones. This feature is connected with difference in the geometry exclusion effects. Blocking of the substrate area is enhanced by the growth of the k-mer length, making the surface more porous. The porosity of the surface is also responsible for the decrease of θ_p with the length of the angled objects (B) from Table I. On the other hand, for compact objects, such as triangles (C) and rhombuses (D), percolation threshold increases with their size. This is the consequence of a low connectivity of these objects.

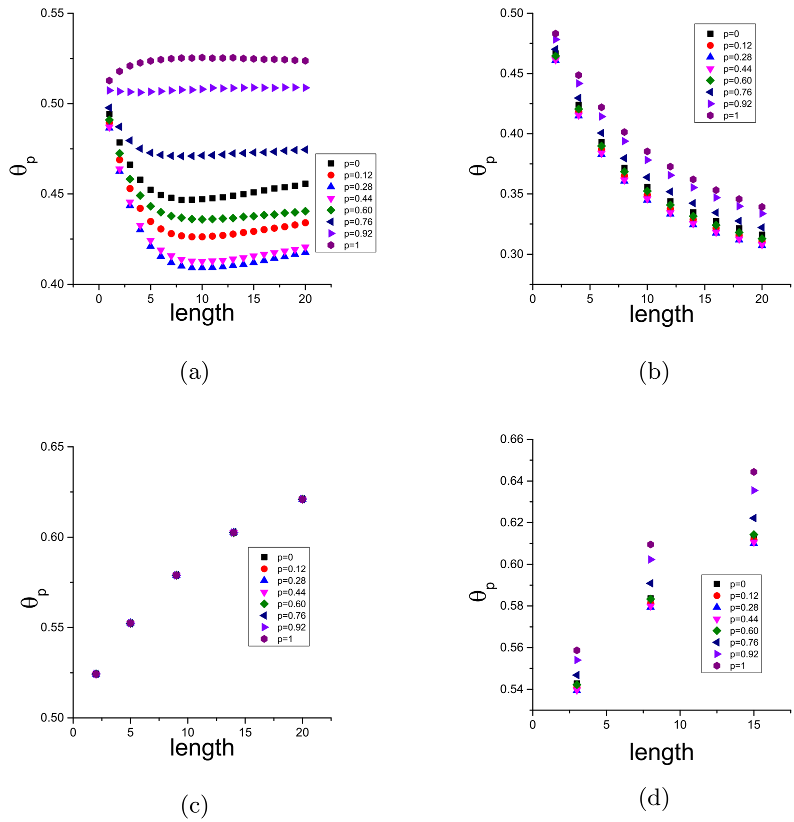


FIG. 2: Dependence of the percolation threshold θ_p on the length of various objects from Table I:
a) (A); b) (B); c) (C); d) (D); for the values of the order parameter:
$p = 0$; 0.12; 0.28; 0.44; 0.60; 0.76; 0.92 and 1.

4. Concluding remarks

Percolation properties in irreversible deposition under anisotropic conditions substrates have been investigated. Objects of various shapes were examined and percolation thresholds were determined for numerous degrees of deposition anisotropy characterized by the order parameter p taking values from $p = 0$ to $p = 1$. It was found that the percolation threshold increases with the degree of anisotropy and have the maximum values for fully oriented objects in one direction. The relative increase of the percolation threshold for the maximum anisotropy ($p = 1$), compared to the isotropic case ($p = 1/3$), is largest for k-mers of length $\ell = 11$. k-mers are these that give the lowest value of θ_p in the isotropic case. On the contrary, percolation of the triangles with the symmetry axis of third order, is not affected by the anisotropy of the underlying lattice.

Crucial difference in the percolation properties of elongated and compact objects was also found. High porosity of the deposit and the high connectivity of elongated objects result in low percolation thresholds for the isotropic, as well as for the anisotropic deposition. θ_p decreases with the size for these objects. On the other hand, low connectivity of the compact objects, like triangles and rhombuses, results in higher percolation thresholds, while θ_p increases with the object size. (It should be noted that the k-mers show a more complex behavior. For the isotropic case θ_p decreases with ℓ for shorter k-mers, reaches a minimum, and increases for longer k-mers. In the presence of anisotropy the minimum is shifted towards shorter k-mers. For highly anisotropic deposition, percolation threshold practically does not depend on the k-mer length.)

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