

# Influence of anisotropy on percolation and jamming of linear $k$ -mers on square lattice with defects

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**Abstract.** By means of the Monte Carlo simulation, we study the layers produced by the random sequential adsorption of the linear rigid objects ( $k$ -mers also known as rigid or stiff rods, sticks, needles) onto the square lattice with defects in the presence of an external field. The value of  $k$  varies from 2 to 32. The point defects randomly and uniformly placed on the substrate hinder adsorption of the elongated objects. The external field affects isotropic deposition of the particles, consequently the deposited layers are anisotropic. We study the influence of the defect concentration, the length of the objects, and the external field on the percolation threshold and the jamming concentration. Our main findings are (i) the critical defect concentration at which the percolation never occurs even at jammed state decreases for short  $k$ -mers ( $k < 16$ ) and increases for long  $k$ -mers ( $k > 16$ ) as anisotropy increases, (ii) the corresponding critical  $k$ -mer concentration decreases with anisotropy growth, (iii) the jamming concentration decreases drastically with growth of  $k$ -mer length for any anisotropy, (iv) for short  $k$ -mers, the percolation threshold is almost insensitive to the defect concentration for any anisotropy.

## 1. Introduction

Deposition of large particles such as colloids, polymers or nanotubes on substrates can be considered and studied as the random sequential adsorption (RSA) [1]. In RSA, objects randomly deposit on a substrate; this process is irreversible, and the newly placed objects cannot overlap or pass through the previously deposited ones. The substrate may be prepatterned (e.g., see [2]) or include some impurities (defects) (e.g., see [3]). The adsorbed objects may be identical or present a mixture of objects of different sizes and shapes (e.g., see [4, 5]). Moreover, anisotropy can be introduced by postulating unequal probabilities for deposition of elongated objects along different directions (e.g., see [5, 6]). The anisotropy of deposition can reflect the influence of the external fields, flows or anisotropy of the substrate. The adsorption of the elongated particles in the presence of the external fields produces the anisotropic layers (e.g., see [7, 8]).

Very often in RSA, a substrate is considered as a discrete space, e.g., regular or irregular lattice, a tree. The simplest, but the most commonly used instance of the discrete substrate is the square lattice. The linear segments are used very often as the objects adsorbed onto the square lattice. The linear segment (also denoted as needle, linear chain, stiff rod or  $k$ -mer) consists of  $k$  successive connected sites.



If the deposition of the objects goes infinitely long, a jamming state is reached. At the jamming state, there are still voids between the previously placed object on the substrate, but their size and shape are not sufficient to deposit even one additional object.

*Definitions.* For a perfect lattice (a lattice without any defects), the jamming concentration,  $p_j$ , is the fraction of the sites occupied by deposited objects. For a diluted (disordered, disturbed) lattice (a lattice with the defects or impurities), there are several ways to define the jamming concentration.

- (i) The jamming concentration,  $\rho$ , is the fraction of all occupied sites, i.e. the fraction of the sites occupied by the deposited objects plus the fraction of the sites occupied by the impurities [9].
- (ii) The pure object jamming limit,  $p_j$ , is defined as the fraction of total lattice sites occupied by the deposited objects [10]. This quantity equals  $\rho - d$ , where  $d$  means the fraction of the sites occupied by impurities.
- (iii) The jamming concentration,  $c_j$ , in terms by Cornette et al. [11], is the fraction of the sites free of the impurities and occupied by the objects, i.e.,

$$c_j = \frac{p_j}{1 - d} = \frac{\rho - d}{1 - d}.$$

In the present research, we utilize everywhere the pure object jamming limit and denote it as the jamming concentration,  $p_j$ , for short.

Ben-Naim and Krapivsky obtained an important analytical result for the one-dimensional case [9]. Initially, a one-dimensional lattice is occupied by the point impurities with the uniform random distribution. Next, the linear  $k$ -mers randomly and sequentially adsorb on the lattice. In this case, the jamming concentration,  $\rho$ , is

$$\rho = d + k(1 - d)^k \int_0^\infty \exp\left(-t - 2 \sum_{i=1}^{k-1} \frac{1 - \exp(-it)}{i} (1 - d)^i\right) dt, \quad (1)$$

where  $d$  is the initial concentration of the point impurities,  $k$  is the length of the objects [9].

If the concentration of the deposited objects on the substrate is sufficiently large, there may be a path through the objects from one side of the system to its opposite side. Below this concentration, there is no spanning path through the system, while above this concentration, there is a connected component of the order of the system size. This concentration is called the percolation threshold. (See, e.g., [12] for the details; art of the state may be found, e.g., in [13].) For the some systems, the percolation never occurs even at the jamming concentration (e.g., the adsorbed layer produced by the deposition of the equal squares on a square lattice if the side of the square is greater than 3 sites [14]). In fact, the percolation threshold corresponds to a phase transition, e.g., insulator-conductor. Different definitions of the percolation threshold are utilized for the lattices with defects similar to the definitions of the jamming concentration. In the present research, we use the term 'the percolation threshold' ( $p_c$ ) as the ration of the sites occupied by the objects to the whole number of the lattice sites.

Cornette et al. [11, 15] investigated numerically the percolation of the polyatomic species in the presence of impurities on a square lattice with periodic boundary conditions. Bond and site percolation problem have been taken in consideration. Linear  $k$ -mers as well so called SAW  $k$ -mers, i.e. segments of self avoiding walk, have been studied up to  $k = 9$ . Phase diagram where the critical concentration of impurities is plotted as a function of  $k$  has been offered.

The kinetics of the random sequential adsorption of line  $k$ -mers (values of  $k$  vary up to 64) has been studied on a disordered substrate occupied by the point impurities [10]. The coverage of

the surface and the jamming limits are calculated by a Monte Carlo method. The coverage has an asymptotically exponential behaviour at low concentration of the impurities. The jamming limits depend on the concentration of the impurities  $d$ . At  $d < d^*$  the jamming limits increase as  $d$  increases. At  $d > d^*$  the jamming limits increase as  $d$  increases, where the value of  $d^*$  depends on  $k$ . In one-dimensional case, the results are in good agreement with published analytic results [9]. The coverage and the jamming limits on a two-dimensional disordered lattice are similar to the one-dimensional case. The jamming limits decrease monotonically as the length of line segments increases. The minimum locations of the jamming limits for both one and two dimensions are on the same values for a given length of the  $k$ -mer.

The effect of anisotropic deposition on the jamming [16] and the percolation [17] was intensively studied by means of the Monte Carlo simulation.

Recently, impact of defects on percolation in random sequential adsorption of linear  $k$ -mers on square lattices was investigated for rather wide range of  $k$ -mers (the length of the  $k$ -mers varies from 2 to 256) [18]. Two different cases were studied: (1) it was assumed that the initial square lattice is nonideal and some fraction of sites  $d$  is occupied by nonconducting point defects (impurities); (2) it was assumed that some fraction of the sites in the  $k$ -mers  $d$  consists of defects, i.e., is nonconducting, whereas the initial square lattice is perfect.

Mixed site-bond percolation was studied for RSA of  $k$ -mers on heterogeneous lattices with of variable connectivity  $z$  [19]. The simulations were performed for  $k = 1-3$  on a triangular lattice. The percolation phase diagrams in terms of the percolation threshold  $p_c$  versus lattice connectivity  $z$  were obtained. For RSA deposition of monomer onto triangle lattice with defects preliminarily filled with  $k$ -mers, the percolation ( $k = 3-24$ ) [20] and the jamming ( $k \leq 50$ ) [21] were investigated by means of the Monte Carlo simulations. The nonmonotonicity of the percolation threshold as a function of the impurity concentration was observed [20].

RSA of polydisperse mixtures of  $k$ -mers was also intensively investigated [5, 22, 23]. A phase diagram separating a percolating from a non-percolating region for mixtures of monomers and  $k$ -mers on a square lattice ( $k = 2-7$ ) was determined [22]. The jamming coverage for a mixture was greater than either of the jamming coverage of the components making the mixture [5]. From other hand the percolation threshold for a mixture was slightly greater than that of the longest  $k$ -mer [23].

Recently, continuum random sequential adsorption of polymer on a flat and homogeneous surface was studied [24].

Our goal is to study the influence of the anisotropy on the percolation threshold and the jamming concentration of the linear  $k$ -mers onto the square lattice with the point defects.

The rest of the paper is organized as follows. Section 2 describes our models of the  $k$ -mer deposition onto a square lattice. The results obtained using finite size scaling theory and dependencies of the percolation threshold,  $p_c$ , and the jamming concentration,  $p_j$ , vs order parameter,  $s$ , and the defect concentration,  $d$ , are examined and discussed in details in Section 3. We summarize the results and conclude the paper in Section 4.

## 2. Method

### 2.1. Anisotropy

To describe the anisotropy, we used the quantity

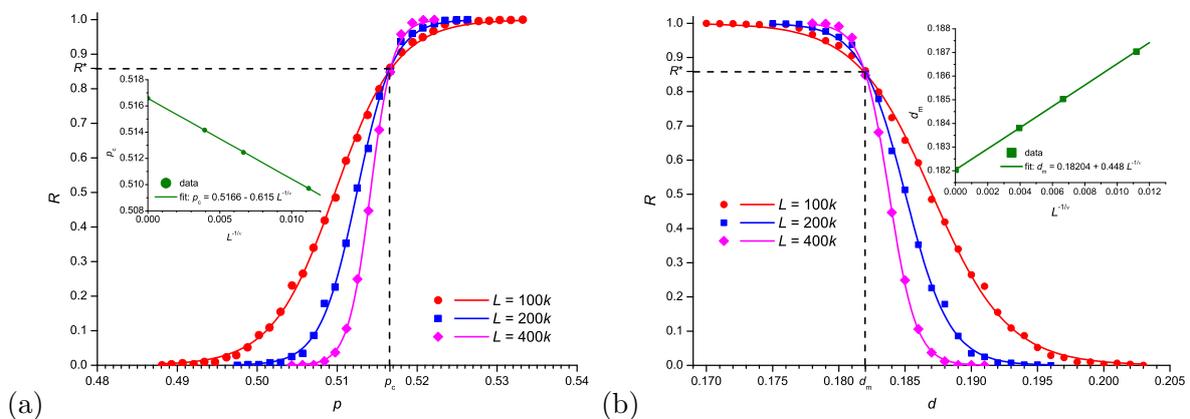
$$s = \frac{|N_{\uparrow} - N_{\downarrow}|}{N_{\uparrow} + N_{\downarrow}}, \quad (2)$$

where  $N_{\uparrow}$  is the number of vertically oriented objects,  $N_{\downarrow}$  is the number of horizontally oriented objects.

### 2.2. Relaxation Random Sequential Adsorption

In our simulation, we utilized the modification of RSA, so-called relaxation random sequential adsorption (RRSA) [16]. In this model, the lattice site is randomly selected and an attempt of deposition of a  $k$ -mer with the orientation defined by the order parameter  $s$  is done. If the attempt is unsuccessful, a new lattice site is randomly selected until the object will be deposited. The objects may move all over the substrate searching for a sufficiently large empty space. The deposition terminates when a jamming state is reached along one direction. We considered the lattice with periodic (toroidal) boundary conditions to eliminate the effect of the border and treated the spiral clusters as wrapping (percolating) in contrast with [25]. We checked the percolation in two perpendicular directions and used two criteria: there is percolation in both directions (criterion AND), there is percolation at least along one direction (OR).

For each given anisotropy,  $s$ , and the concentration of the defects,  $d$ , we filled the lattice with the  $k$ -mers to the concentration  $p$  or to the jamming and checked whether the percolation. We repeated it 1000 times and found the probability,  $R(p)$ , that the percolation occurs at given concentration of the  $k$ -mers. The abscissa of the inflection point of the curve is treated as the estimation of the percolation threshold for the given lattice size. We used the lattices of the sizes  $L = 100k, 200k, 400k$  and performed finite-size analysis to obtain the percolation threshold in the thermodynamic limit ( $L \rightarrow \infty$ )  $p_c \propto L^{-1/\nu}$ , where the critical exponent  $\nu = 4/3$  [12]. All probability curves intersect each other in one point with the co-ordinates  $(p_c, R^*)$ , where  $R^* = R(p_c) \approx 0.859$ . The value of  $R^*$  depends on how the percolation is defined [25]. The intersection point offers another way to estimate the percolation threshold. Examples of probability curves and scaling are shown in Fig. 1.



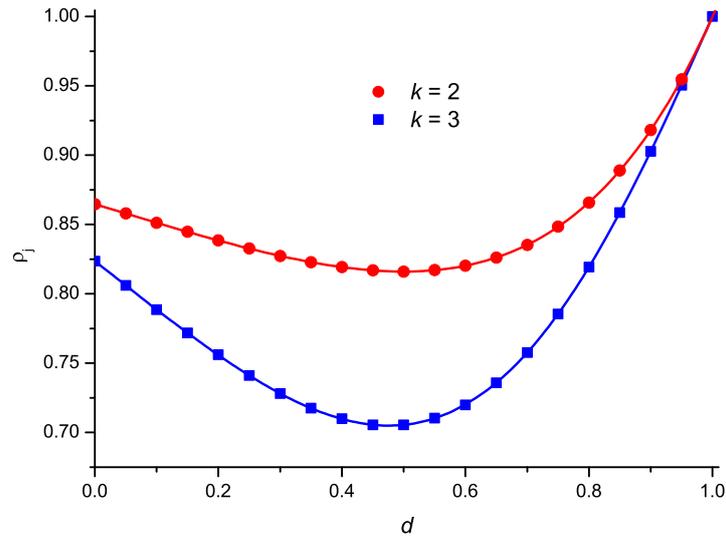
**Figure 1.** The probability curves for  $k = 4$ ,  $s = 0.5$ . (a)  $R(p)$ . (b)  $R(d)$ . Insets: scaling. The statistical error is smaller than the marker size.

We compared our numerical simulation for completely aligned  $k$ -mers ( $s = 1$ ) with the analytical results [9]. Figure 2 shows that there is not any visible difference between analytical and numerical results.

### 3. Results

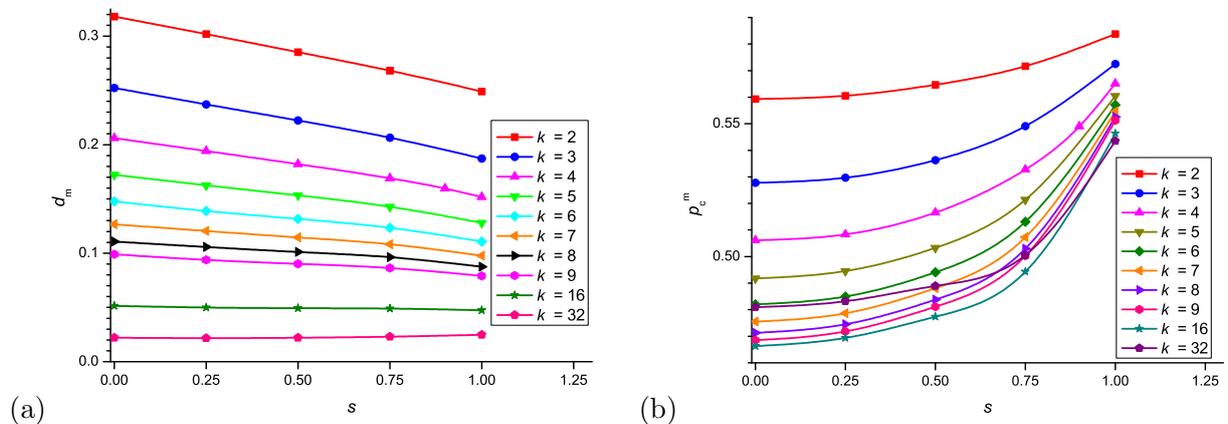
We denote as  $d_m$  the critical defect concentration, i.e. the defect concentration above which the percolation never occurs even at jammed state. We denote as  $p_c^m$  the critical  $k$ -mer concentration for given concentration of defects, i.e. the object concentration at which the percolation occurs at jammed state only.

The critical defect concentration,  $d_m$ , decreases for short  $k$ -mers ( $k < 16$ ) and increases for long  $k$ -mers ( $k > 16$ ) as anisotropy,  $s$ , increases (see Figure 3a). The critical  $k$ -mer concentration,



**Figure 2.** The total jamming coverage,  $\rho_j$ , for completely aligned ( $s = 1$ ) dimers ( $k = 2$ ) and trimers ( $k = 3$ ) as a function of the concentration of point defects,  $d$ : theory (1) (lines) and our numerical simulations (symbols). The statistical error is smaller than the marker size.

$p_c^m$ , decreases with anisotropy growth (see Figure 3b). It looks like, this dependence may be nonmonotonic and have a minimum somewhere about  $s \approx 0.5$  for long objects ( $k > 32$ ).



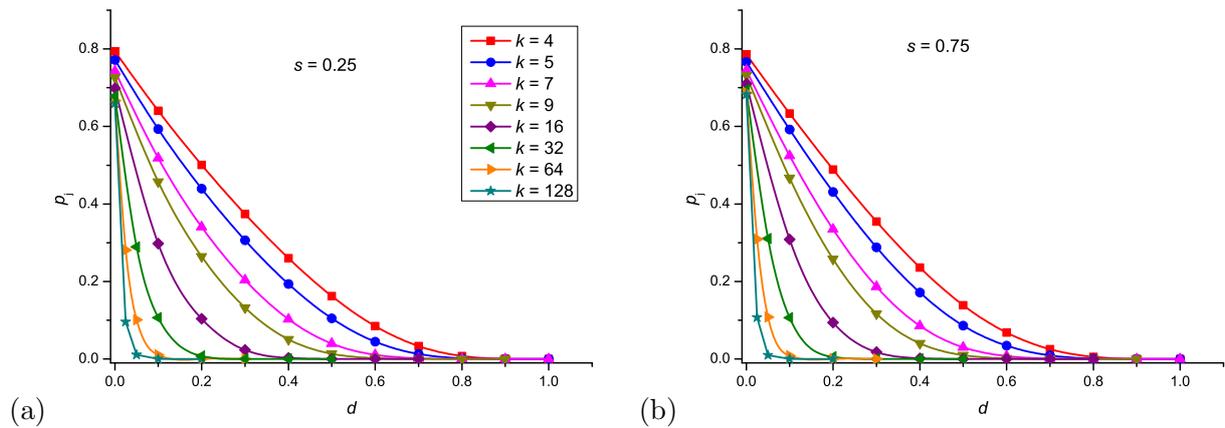
**Figure 3.** (a) The critical defect concentration,  $d_m$ , and (b) the critical  $k$ -mer concentration,  $p_c^m$ , as a function of anisotropy,  $s$ , for different length of the  $k$ -mers. The solid lines are a guide to the eye. The statistical error is smaller than the marker size.

The jamming concentration decreases drastically with growth of  $k$ -mer length for any anisotropy (see the samples for  $s = 0.25$  and  $0.75$  in Figure 4).

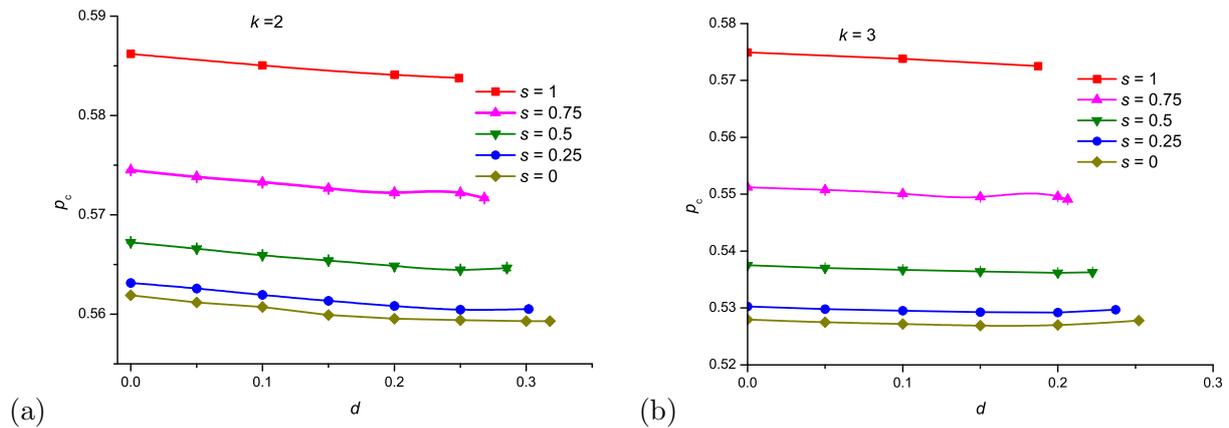
For short  $k$ -mers, the percolation threshold,  $p_c$ , is almost insensitive to the defect concentration,  $d$ , for any anisotropy,  $s$  (see Figures 5).

#### 4. Conclusion

In our work, the percolation and jamming behavior of partially ordered linear  $k$ -mers on a square lattice with periodic (toroidal) boundary conditions has been investigated by computer



**Figure 4.** The jamming concentration,  $p_j$ , as a function of the defect concentration,  $d$ , for different  $k$  and fixed anisotropy (a)  $s = 0.25$ , (b)  $s = 0.75$ . The solid lines are a guide to the eye. The statistical error is smaller than the marker size.



**Figure 5.** The percolation threshold,  $p_c$ , as a function of the defect concentration,  $d$ , for different anisotropy,  $s$ , for (a) dimers ( $k = 2$ ) and (b) trimers ( $k = 3$ ). The solid lines are a guide to the eye. The statistical error is smaller than the marker size.

simulations. The lattice is imperfect, i.e. some fraction of the lattice sites is occupied by defects (impurities). The length of a  $k$ -mer varies from 1 to 32. The relaxation random sequential adsorption model [16] has been used to deposit the  $k$ -mers with the given anisotropy. The anisotropy is characterized by order parameter  $s = 0 \dots 1$ , where  $s = 0$  corresponds to the isotropic system and  $s = 1$  corresponds to the system with completely aligned objects. The defects hinder the adsorption of the elongated objects. If the concentration of the defect exceeds the critical value,  $d_m$ , the percolation cannot occur. The dependence of critical concentration on anisotropy,  $d_m(s)$ , is almost linear function for any value of  $k$ . Even a small concentration of the defects inhibits the deposition of long objects. Additional studies with long objects ( $k > 32$ ) look promising because the real objects of practical interest (e.g., nanotubes), can have large aspect ratios.

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