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Percolation and jamming properties in limited grain growth of linear objects

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Abstract: The physical and chemical properties of the nanocrystals are highly shape dependent, and shape control has become very important. The seeded growth method enables seeds to grow in a predetermined way. We have already proposed such a model that can reproduce the granular growth on a triangular lattice and for different growth shapes. In this paper, however, we have introduced a limitation on seed growth up to a certain length. This method can be used when the growth of all seeds have to be limited to the same length, or for a mixture with the different growth limits. The main goal is to investigate how the growing limits affect the values of the percolation threshold and jamming density, and whether large objects significantly affect the percolation threshold. We used growing needle-shaped objects (k-mers) made by a self-avoiding random walk filling the nodes of the triangular lattice. Objects can grow until they reach the growth limit k' defined as the maximum number of lattice nodes belonging to one object. For $k' \geq 10$, percolation is reached for all investigated seed densities. We obtained that the values of the percolation threshold and jamming density are identical for $k' \geq 10$. Above these values, the percolation threshold and jamming remain unchanged, regardless of the growth limit. Our results also show that when significant growth is allowed, long objects are very rare and do not influence the results.

INTRODUCTION

Percolation is a second-order phase transition. The study of percolation started with the work of the chemist P. Flory in his study on gelation in polymers (Flory, 1941). The percolation theory deals with the clusters formed when each site of an infinite lattice is randomly occupied with probability p (Staufer & Aharony, 1994). A cluster (groups of neighbouring occupied sites) that connects two opposite lattice sides is called a percolation cluster, and it will appear when the probability p reaches a critical value p_c, which is called the percolation threshold (Hao, 2005). Finding the percolation threshold for a given system is one of the fundamental tasks. Percolation is used to explain, for example, the gelation of polymeric materials (Stauffer, Coniglio and Adam, 1982). the growth of rough surfaces and disordered interfaces via atomic chemisorption (Meakin, 1993), the recovery of oil from porous media (King, Buldyrev, Dokholyan, et al., 2002), ion transport in glasses and composites (Roman, Bunde, and Dieterich, 1986).

In standard percolation theory, the constituent elements of the clusters are usually randomly distributed, but correlations cannot always be neglected. Several correlated percolation models have been developed and extensively studied, such as bootstrap percolation (Adler, 1991), directed percolation (Broadbent & Hammersley, 1957), and spiral percolation (Santrs & Bose, 1992).

In the last two decades, it has become possible to synthesize many classes of nanoscale building blocks with controlled structure, size, and shape for applications in chemical engineering, medicine, electronics, etc. Seeded growth has emerged as a compelling method to create a wide variety of novel metal nanostructures (Gole & Murphy, 2004); Habas, Lee, Radmilovic, et al., 2007) and high-quality nanocrystal samples that can serve as preferential platforms for deposition of additional material (Xia, Gilroy, Peng, et al., 2017). Dujak, Karač, Budinski-Petković, et al., (2022), proposed a model that can reproduce granular growth on a triangular lattice, from nucleation to percolation, and for different growing shapes. The object's growth was not limited. In this paper, we investigate how the growth limit of the needle-like objects (k-mers) affects the values of the percolation threshold and the jamming density.

EXPERIMENTAL

Definition of the model and the simulation method

The Monte Carlo simulations are performed on a two-dimensional triangular lattice of different sizes L. Periodic boundary conditions are used. Coverage of the lattice $\theta(t)$ is the fraction of the covered lattice sites by the growing objects at time t. At large times the coverage $\theta(t)$ approaches the jammed-state value called jamming coverage θ_J. In that state, none of the objects can grow to unocupied spaces. The percolation threshold θ_p^* is the coverage of the lattice when a percolating cluster appears. The lattice is filled with objects using random sequential adsorption model (RSA) (Evans, 1993), (Privman, 2000) (Cadilhe, Araújo, and Privman, 2007). The growing objects on the lattice are modeled by self-awoiding walks (Budinski-Petković, Lončarević, Dujak, et al., 2017)

Definition of the model

The point-like seeds are deposited on the sites of the planar triangular lattice at a given density ρ. Density of seeds is calculated as a fraction of sites of the lattice that are occupied by seeds. Each seed can grow only in one direction, creating a linear object called k-mer. K-mers are line-segments of lenght $l = k - 1$ where k denotes the number of the lattice sites that belongs to that particular k-mer. The formation of k-mers with corresponding percolation thresholds and jamming coverages is shown in Table I.

Table I: Formation of k-mers of different lengths $l = k - 1$ (up to $l = 3$) with corresponding percolation thresholds θ_p^* for infinitely large lattice and jamming coverages θ_J. The numbers in parentheses are the numerical values of the standard uncertainty of θ_p^* and θ_J referred to the last digits of the quoted value.

k-mer	k	l	θ_p^*	θ_J
●	1	0	0.5000(1)	1
●—●	2	1	0.4867(1)	0.9141(3)
●—●—●	3	2	0.4628(3)	0.8362(4)
●—●—●—●	4	3	0.4432(2)	0.7891(6)

As the k-mers grow, they come in contact (i.e. there is a lattice site between them) and they are merged into a single cluster. There are numerous clusters that grow simultaneously. If two clusters come into contact (i.e. occupied perimeter sites are separated by a single lattice spacing), they are amalgamated into a single cluster. Percolation is reached when a cluster connects opposite edges of the lattice and then the percolation threshold θ_p^* is reached. To determine the percolation threshold θ_p^*, the tree-based union/find algorithm is used (Newman & Zi, 2001). The jamming coverage θ_J is reached when no more growing objects can grow in growing direction on the lattice (Lončarević, Budinski-Petković and Vrhovac, 2007; Budinski-Petković, Vrhovac, and Lončarević, 2008).

Simulation method

The RSA model of seeds in two dimensions is used to prepare the initial state of the system. Monomers (k-mers with $k = 1$) that represent the point-like seeds are deposited onto lattice using the Monte Carlo procedure, up to the chosen density ρ. Then deposition is switched off and a random growing process is initiated.

At each Monte Carlo step, a lattice site occupied by seed is selected at random. An adjacent site that is not occupied by another seed or k-mer is selected randomly and the seed grows into dimer (k-mer with $k = 2$). A double occupation at any site is not allowed. Only a single step k-mer growth is allowed and only the last point of the corresponding k-mer is active for further growth. The k-mers can grow only in direction of the first step. If the corresponding adjacent site is not empty, the k-mer elongation attempt is not possible and the object remains unchanged. The growth of the k-mers is limited up to k' i.e. they can grow until they reach the lenght $l = k' - 1$ defined at the beginig of the simulation.

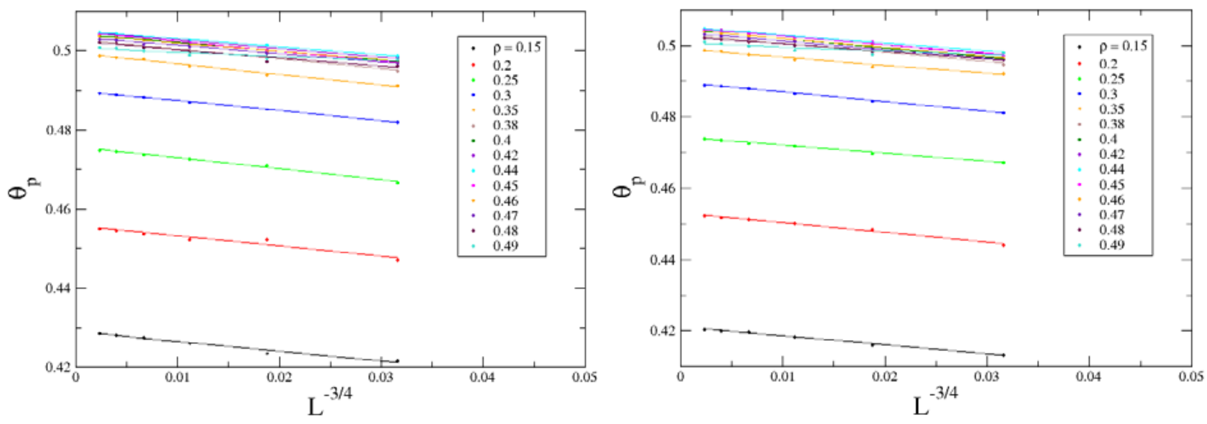
RESULTS AND DISCUSSION

The percolation threshold and jamming coverage were investigated for various seed densities $0.15 \leq \rho \leq 0.49$ on the lattice size ranging from $L = 100$ to $L = 3200$, and for various growth limits $2 \leq k' \leq 160$. The data are averaged over 500 independent runs for each lattice size.

The finite-size scaling theory of the percolation behavior on two-dimensional lattices (Staufer & Aharony, 1994) is used to obtain the percolation threshold for un infinitely large lattice θ_p^*. According to this theory, the efective percolation threshold θ_p (the mean value of threshold measured for the finite lattice) approaches the asymptotic value $\theta_p \to \theta_p^*$ for $L \to \infty$ via the power law:

$$\theta_p - \theta_p^* \propto L^{-1/\nu} \qquad (1)$$

where the constant $\nu = 4/3$ is the critical exponent (Staufer & Aharony, 1994). Equation (1) allows extrapolation of the threshold for an infinite lattice. Finite-size scaling of the lattice threshold θ_p against $L^{-3/4}$ is shown in Figure 1.a and Figure 1.b for various initial seed densities and for $k' = 4$ and $k' = 160$ as representatives.



(a) (b)

Figure 1: Finite-size scaling of the effective percolation threshold θ_p against $L^{-1/\nu}$ with $\nu = 4/3$ for growing k-mers up to a) $k' = 4$, b) $k' = 160$

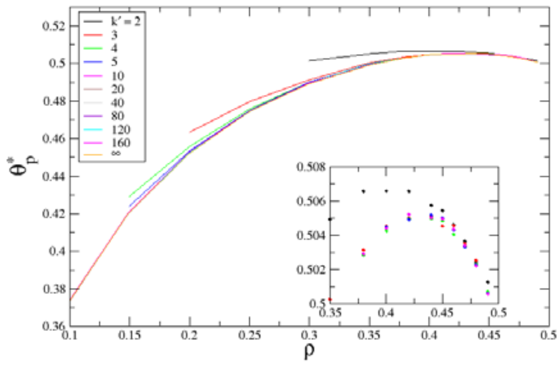


Figure 2: Dependence of the percolation threshold θ_p^* on the initial seed density ρ. The inset shows an enlarged part of this graph that displays a non-monotonic behaviour for $k' = 2, 3, 4, 5, 10$

The dependence of the percolation threshold θ_p^* on the initial seed density ρ is shown in Figure 2. It can be seen that the percolation is not reached for all seed densities depending on the growth limits k'. If $k' = 2$, the percolation is reached for $\rho \geq 0.3$, if $k' = 3$ the percolation is reached for $\rho \geq 0.2$, and for $k' = 4$ and 5 the percolation appears at $\rho \geq 0.15$. For $k' \geq 10$ the percolation was achieved for all investigated densities. However, for all k' the percolation threshold increases monotonically for low values of seed density, reaches a maximum for seed densities in the interval $0.4 < \rho < 0.45$, and then for higher values of seed density, θ_p^* decreases for all k' towards the same value $\theta_p^* = 0.5$. The results for $k' \leq 5$ differ slightly from each other showing a little bit higher values of θ_p^* for the same seed densities. For $k' \geq 10$ the results overlap.

At low values of initial seed densities, k-mers have enough space to grow, but if their growth is limited to small lengths, the surface remains very porous, and a percolation cluster can not be formed. On the other hand, if a percolating cluster is reached, the percolation threshold θ_p^* will have higher values for lower values of the growth limits k'.

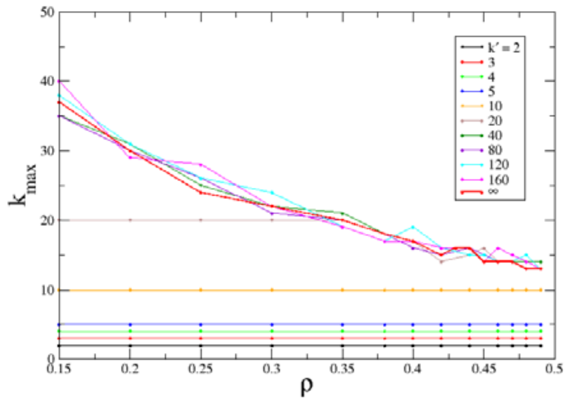


Figure 3: Largest growing objects in the jamming coverages vs. the initial seed density ρ on the lattice sizes $L = 3200$.

The maximum reached lenght limits depending on the seed density, for different growth limits is shown in Figure 3. For $k' < 20$ the set growth limit is reached for all seed densities. For $k' \geq 20$ there are critical maximum lengths of k-mer growth regardless of growth limit k', depending only on the initial density of seeds. When significant growth is allowed, long objects are very rare and do not influence results.

Unlike the results shown in Figure 3, where the mean value of the maximum length reached at least once in all 500 independent simulations is shown, Figure 4 shows the mean value of the maximum length $\bar{l}_{max}$ of the k-mers in all 500 independent simulations. It is obvious that in the cases where the k-mers have not reached the growth limit, the mean value of the maximum length is identical for all growth limits.

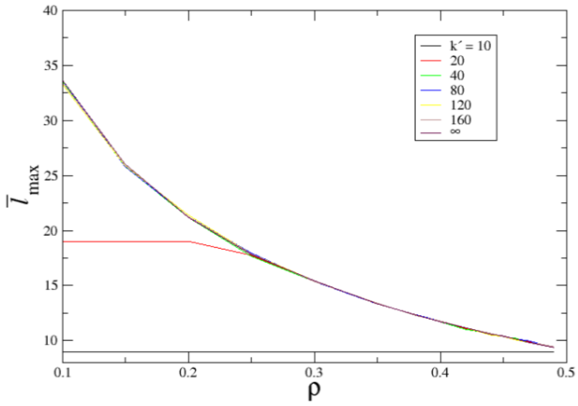


Figure 4: The mean value of the maximum length $\bar{l}_{max}$ for different seed densities ρ and growth limits k'. For $k' < 10$, $\bar{l}_{max}$ is always equal to $k' - 1$. Size of the lattice is $L = 3200$.

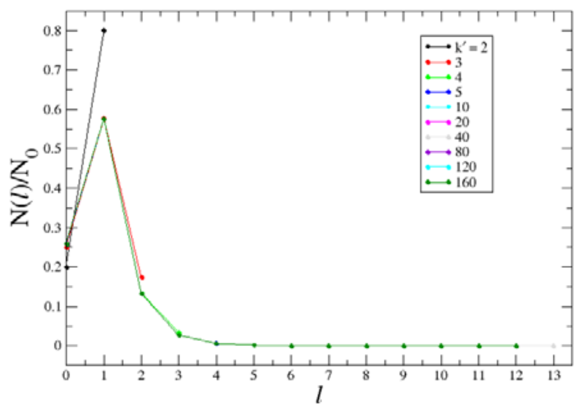


Figure 5: Dependence of the normalized number of deposited k-mers $N(l)/N_0$ on the k-mers length l, for the system in the jamming state. The results are given for seed density $\rho = 0.49$ on the lattice sizes $L = 3200$, for different k' indicated in the legend. Here, N_0 is an initial number of seeds at a given density ρ.

Figure 5 shows the dependence of the normalized number of deposited k-mers $N(l)/N_0$ on their length l. It can be seen that the results for the growth limit $k' \geq 10$ are almost identical (the results are slightly different for $k' \geq 5$ which is not noticeable in this graph).

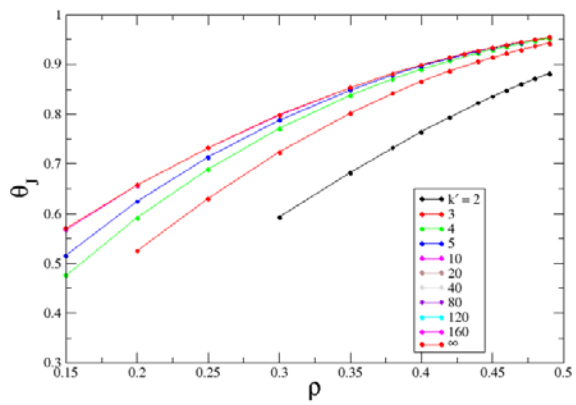


Figure 6: Dependence of the jamming coverage θ_J on the initial seed density ρ for growing k-mers.

They differ only in the maximum length reached at $k' = 40$. For larger k-mers, ratio $N(l)/N_0 \to 0$, this means that long k-mers are very rare. In all cases dimers ($k = 2$) are the most numerous k-mers.

The jamming coverage θ_J (for the cases where percolation is reached) for different growth limits and seed densities is shown in Figure 6. For lower values of the growth limit, θ_J has lower values. As the growth limit increases, the values of the jamming coverage for a particular seed density increase and become identical for $k' \geq 10$.

CONCLUSION

Dependence of the percolation threshold and the jamming coverage on the limit of k-mers growth using numerical simulations was investigated. Simulations were performd for initial states with various initial seed densities and for different growth limits.

Depending on the growth limit percolation was not reached for all seed densities. For the lowest value of the growth limit $k' = 2$, the percolation is reached for $\rho \geq 0.3$. When the growth limit increases, the seed density for which percolation appears decreases. For $k' \geq 10$ the percolation was achieved for all investigated densities. For the same seed densities, the values of the percolation threshold for $k' \leq 5$ have a slightly higher values than for $k' \geq 10$. For all growth limits k', the percolation threshold θ_p^* increases with seed density ρ, reaches a broad maximum, and then decreases. The results become identical for $k' \geq 10$.

The jamming coverage θ_J also increases with ρ for all the growth limits, and the values of θ_J become identical also for $k' \geq 10$. For lower values of the growth limit, θ_J has lower values.

The k-mers can reach a given lenght in cases where growth limit is less than 20. For $k' \geq 20$ there are critical maximum lengths of k-mer growth regardless of the growth limit k', depending only on the initial density of seeds but the mean value of the maximum length is identical.

These results suggest that there is a critical growth limit for k-mer growth, above which the percolation threshold and jamming coverage remain unchanged for all seed densities. There are also critical maximal lengths of k-mer growth regardless of the growth limit k', depending only on the initial density of seeds.

Although present, long k-mers, when significant growth is allowed, are very rare and do not influence the results. On the other hand, small k-mers have a significant role that can be further investigated by making a mixture of seeds with two or more different growth limits. It is also interesting to follow the changes in the percolation threshold if some point-like impurities are initially added to the lattice.

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Summary/Sažetak

Fizička i hemijska svojstva nanokristala u velikoj mjeri zavise od njihovog oblika, tako da je kontrola oblika postala veoma važna. Metoda rasta sjemena omogućava sjemenu da raste na unaprijed određen način. Ranije smo predložili model koji može da reprodukuje rast sjemena na triangularnoj rešetki tako da se formiraju različiti oblici. U ovom radu smo, međutim, uveli ograničenje na rast sjemena do određene dužine. Ovaj metod se može koristiti kada je rast svih sjemena ograničen na istu dužinu, ili za smjese sjemena s različitim konačnim dužinama. Glavni cilj je ispitati kako ograničenje rasta utječe na perkolacioni prag i gustinu zagušenja, te ispitati da li dugački objekti značajno utječu na perkolacioni prag. Koristili smo narastajuće objekte u obliku igle ili k-mere koji su formirani samoizbjegavajućim slučajnim šetnjama koje popunjavaju čvorove triangularne rešetke. Objekti mogu da rastu dok ne dostignu granicu rasta k' koja je definisana kao maksimalni broj čvorova rešetke koji pripadaju jednom objektu. Za $k' \geq 10$ perkolacija je postignuta za sve ispitivane početne gustine sjemena. Dobili smo da za granice rasta $k' \geq 10$ vrijednosti perkolacionog praga i gustine zagušenja se preklapaju za sve vrijednosti gustine sjemena. Iznad ovih vrijednosti perkolacioni prag i gustina zagušenja ostaju uvijek isti bez obzira na granicu rasta. Rezultati pokazuju da kada je dozvoljen znatan rast, dugački objekti su veoma rijetki i ne utječu na rezultate.