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Formation of a through conductive inclusion in a layered sample with sector conductive inclusions in single layers. Probability of a through inclusion appearance

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The paper presents the results of studying the formation of a through conductive inclusion in a layered sample for the case of sector conductive inclusions in single layers. The distribution of inclusions in the layers is uniform and independent in different layers. The values of the probability of occurrence of a through conductive inclusion are obtained for various values of the system parameters − the size of inclusions in layers, their number, and the number of layers. The dependences of this probability on the average filling of the layer with the conducting phase are obtained. Percolation threshold values are obtained.
Keywords: Through conductive inclusion, sector inclusions in layers, percolation

Формування наскрізного провідного включення в шаруватому зразку з секторними провідними включеннями в окремих шарах. Імовірність появи наскрізного включення *Р.Є. Бродський, Т.В. Кулик*

У роботі представлені результати дослідження формування наскрізного провідного включення в шаруватому зразку для випадку секторних провідних включень в окремих шарах. Розподіл включень у шарах однорідний і незалежний в різних шарах. Отримано значення ймовірності виникнення наскрізного провідного включення для різних значень параметрів системи − розміру включень у шарах, їх кількості, числа шарів. Отримані залежності цієї ймовірності від середнього заповнення шару провідною фазою. Отримано значення порога перколяції.

1. Introduction

The formation of conducting clusters in the case of a random distribution of the conducting phase in materials is widespread and occurs in various technological processes. The theory of such phenomena is closely related to the theory of percolation. The theory of percolation describes systems with a flow in the broadest sense − the conduction of electric current, the flow of liquids or gases in porous media, the dissemination of information in networks, both electronic and in networks of social, human connections. Despite the active development, a significant number of works in this area appear even now. So, studies on the spread of infections in social networks [1-2], as well as its blocking through immunization [3], are relevant. Studies of percolation in physical systems, including technical [4], natural [5] and biological [6] are ongoing.

Classical approaches to percolation theory include discrete and continuous percolation. In discrete percolation problems, a system is considered as a graph or lattice (for example, a square one), consisting of point nodes and links between them. The approach of discrete percolation on lattices is the most developed, however, it continues to develop [7]. In problems of continuous percolation, the appearance of conductivity in a continuous non-conducting medium with continuous conducting inclusions is studied. In classical problems, round inclusions (in the two-dimensional case) and spherical (in the three-dimensional case) are usually considered; in modern works, percolation with inclusions of other shapes, for example, cylinders [8-11] oriented in one direction or in arbitrary ones, is studied. Percolation in a conducting medium with "excluded" cylinders is also considered.

Modern works on percolation in a system consisting of layers are mainly devoted to multilayer discrete networks [12-16], where discrete nodes are located in each layer, i.e. the discrete problem of percolation is considered. In this paper, conducting inclusions in layers are considered to be continuous.

In this paper, we consider the occurrence of a conducting inclusion in a sample that is continuous in one direction, in the plane of the layers, and discrete in the other, in the direction perpendicular to the layers. In considered case, the characteristic dimensions of the inclusion are comparable with the size of the system, at least in the plane of the layer. This is a significant difference from typical percolation problems. However, determining the probability of occurrence of a conductive inclusion as a function of the control parameters for the formation of individual inclusions will also be one of the central tasks of this work.

In [17], the case of the formation of a through conductive inclusion in a layered sample consisting of round layers was considered, when the inclusions in the layers have the shape of round "islands", the cases of different sizes and numbers of islands and sample layers were considered.

This work is devoted to the study of the case of sector inclusions. Consideration of the case of sectors is interesting for two reasons. On the one hand, they represent tosent physically reasonable problems of radially symmetric inclusions that can form when the layer grows from the center to the edge. On the other hand, they allow you to enter and study one-dimensional models. Such one-dimensional models are extremely useful due to their simplicity, in this case they also turn out to be equivalent to physically realizable problems.

2. Formulation of the problem.

The work is devoted to studing the probability of occurrence of conductivity in a layered sample with conductive sector-type inclusions in single layers. A sample consisting of N layers with n inclusions-sectors in each layeri is considered.

It is easy to see the equivalence of this case to the one-dimensional problem of conducting inclusions-segments in layers-circles. For convenience, we choose the units of measurement of the area of inclusions so that the problem is numerically equivalent to the one-dimensional problem for unit circles (circles of length 1) with segments-inclusions with lengths $l \in (0,1]$. To do this, we take the area of the layer as a unit, then the areas of the sectors-inclusions will be expressed in fractions of the area of the entire layer – in fractions of a unit. Sectors are naturally set by the angle between the radii bounding the sector, we can make such an angular characteristic of the sector also numerically equivalent to the length of the segment-inclusion in a one-dimensional problem and, what is the same, numerically equal to its area, if, under the accepted condition of the unit area of the layer, we measure angle by "natural parameter" – i.e. as a part of total turnover. With these methods of measurement, the angular measure of an inclusion numerically coincides with its area and numerically coincides with the length of the segment in the equivalent one-dimensional problem, both for an individual inclusion and for combined inclusions that will arise when individual inclusions are superimposed in a layer. We will talk about the angular measure or the area of the inclusion or the length of the equivalent segment, depending on the convenience and discriptiveness in a particular context, the same value will be mentioned. Inclusion "size" will be used as a general term for this quantity.

In paper, we consider the case of n inclusion sectors of the same size $r \in (0,1]$ in all layers. The location of inclusions in a layer is random and independent of both the location of other inclusions in the layer and the location of inclusions in other layers.

For a precise definition of the notion of the location of an inclusion, we will accept the following description of the location. A

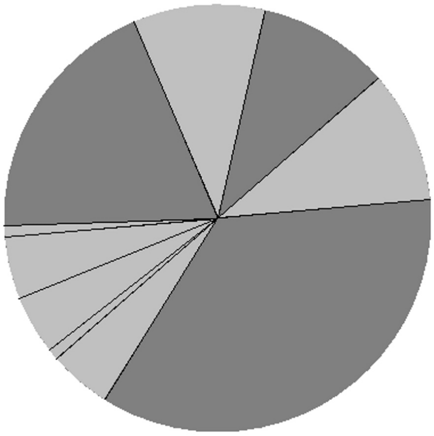

Fig. 1. Example of a layer, showing the non-conductive part, conductive inclusions and their boundaries

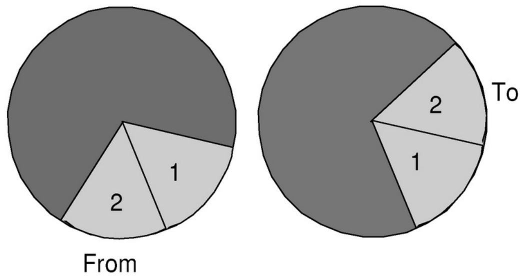

Fig. 2. Limit positions of inclusion 2 relative to inclusion 1, at which there is contact between inclusion

sector inclusion lies between two radii (a segment-inclusion in an equivalent one-dimensional problem lies between two points on a circle). The position of the radius is determined by the angle between the given radius and the given reference direction, which is the same in all layers. The angle is laid counterclockwise. The first one, when moving counterclockwise, the radius bounding the given sector will called the initial or left one, the second - the final or right one. The angle from the initial to the final radius, counted counterclockwise, is the same for any inclusion and is equal to r. By a random and independent position of an inclusion, we mean a random and independent position of its initial radius.

Inclusions can intersect, creating larger inclusions. An example of a layer is shown in Fig. 1.

The conductive part is shown in light gray, the non-conductive part in dark gray, the boundaries of the inclusions are shown with black lines for clarity. The layer contains $n = 5$ inclusions size $r = 0{,}1$. It can be seen that three inclusions have intersected (the boundaries of each can be tracked by measuring the angle seen on non-intersecting inclusions). In the formation of a through conductive inclusion, these three inclusions will participate as one common sector inclusion.

The outer circumference of the layer, if we mark on it the reference points of the radii that bound the sector inclusions, can be considered as an illustration of an equivalent one-dimensional problem, the circumference in this case should be taken as unity.

The system under study consists of N, such layers by n inclusions size r in each, the location of the inclusions is random. If inclusions in single layers, in contact with each other, form a through, from the first to the last layer, conductive channel, the sample as a whole will be conductive. The probability of such a conductive channel depends on N,n,r. The paper studies the dependence of the probability of occurrence of a through conductive inclusion on N,n,r in a wide range of parameter values.

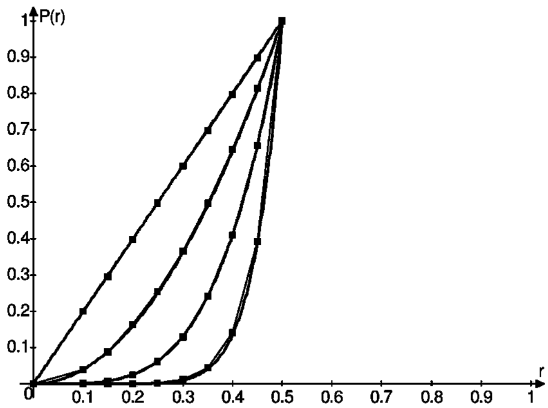

Fig. 3. Probability $P_N(r)$ the occurrence of a through conductive inclusion for $n = 1$ inclusion in layer as a function of size r of inclusion for $N = 2,3,5,10$ from the top graph to the bottom

3. Exactly solvable case.

Although, in the general case the search for the probability of formation of a conductive inclusion requires numerical simulation, for the special case it can be obtained analytically. This is the case only $n = 1$ inclusion in the layer. In this case, the probability of formation of a through conductive inclusion is equal to the probability that there is a contact between a single inclusion in the first layer and in the second, in the second and in the third, and so on. Since

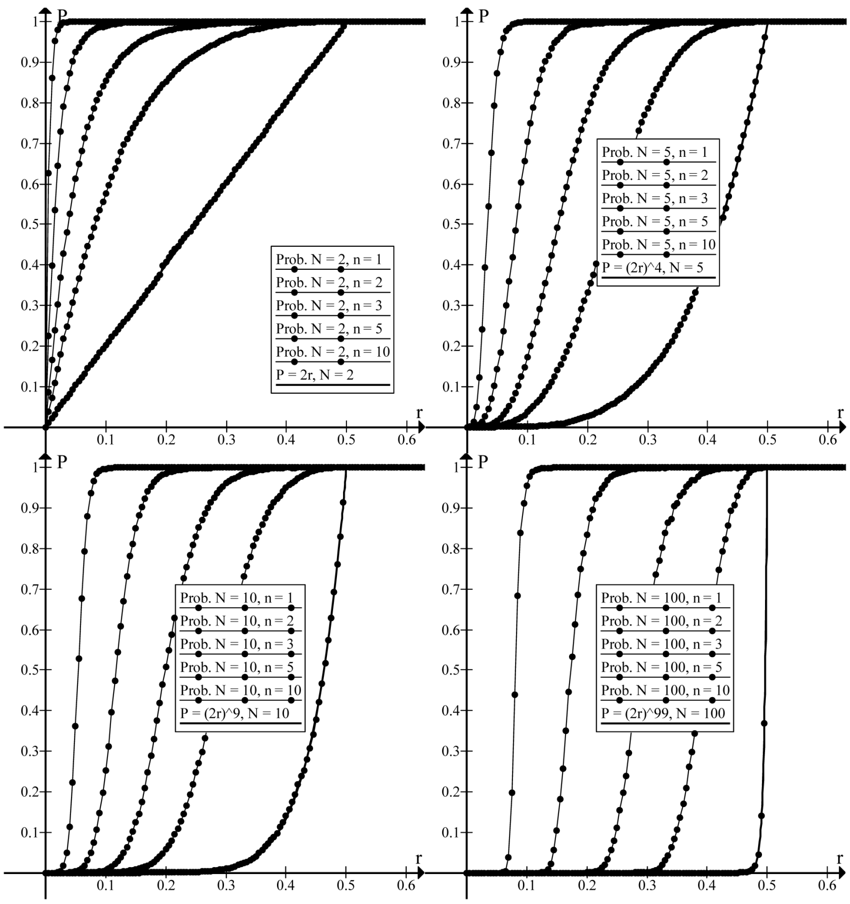

Fig. 4 Probability $P(r)$ formation of a through conductive inclusion in the sample of N layers by n inclusions in each layer as a function of the size of one individual inclusion r. Each fig. matches one value N, left to right and top to bottom $N = 2,5,10,100$, each graph in fig. matches one value n, graphs from right to left match $n = 1,2,3,5,10$.

the position of the inclusion in each layer is random, uniform over the layer (along the angle) and independently in all layers, the probability of contact between inclusions in adjacent layers is the same for any two adjacent layers, therefore, denoting for this case the probability of forming a through conductive inclusion in all sample from N layers depending on the inclusion size r as $P_N(r)$ and the probability of contact between inclusions in two adjacent layers (coinciding with the probability of forming a through conductive inclusion for the case $N = 2$) $P_2(r)$, for this special case we have

$$P_N(r) = \left(P_2(r)\right)^{N-1}$$

Probability $P_2(r)$ for $r>0,5$ is equal to one – two sectors with an opening angle greater than 180^0 must have an intersection. For $r \le 0,5$ the probability of contact can be found from the following considerations. Let the sector-inclusion in one layer be located between the radii at the angles φ and $\varphi + r$. Then the initial radius of the sector in the neighboring layer, in order for the sector to have contact with the neighboring one, must be located from $\varphi - r$ to $\varphi + r$ (Fig.2), i.e. at any angle within a length interval $2r$.

Since the sectors in the layer are evenly distributed, the probability that the second sector will be, i.e. its left radius will be in the interval $2r$ in units of a natural parameter, where a full turn corresponds to one, $P_2(r)=2r$.

Thus, the probability of the formation of a through conductive inclusion in the sample of N layers with a single inclusion size $r \le 0,5$ in each is equal

$$P_N(r)=(2r)^{N-1}$$

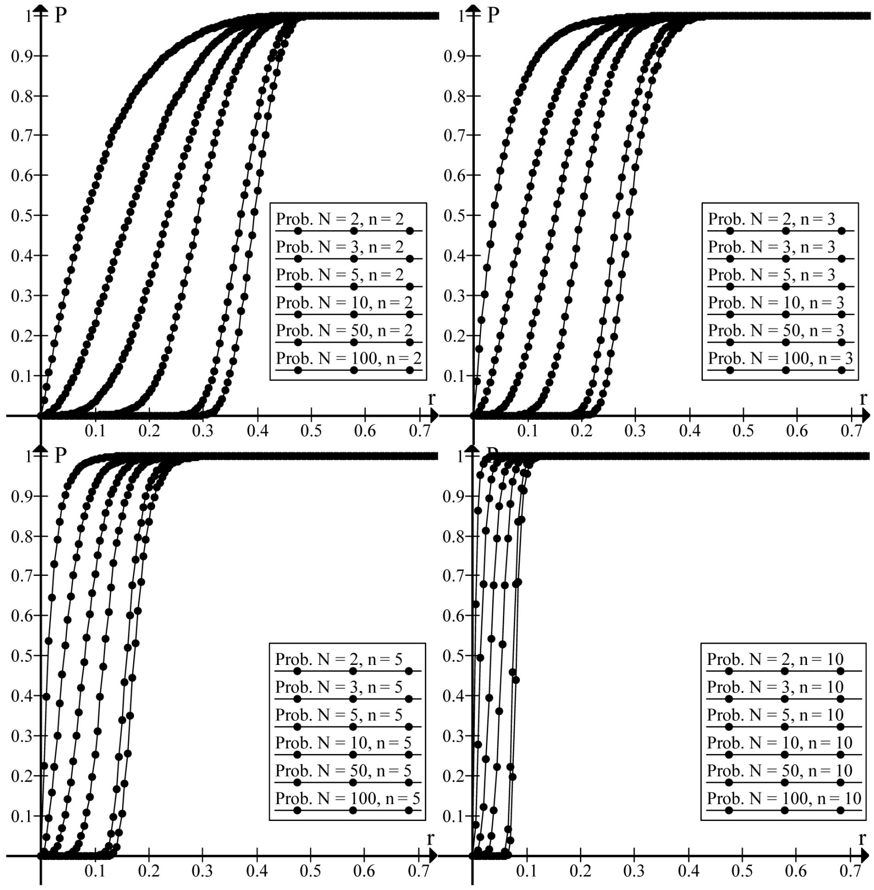

Fig. 5 Probability $P(r)$ formation of a through conductive inclusion in the sample of N layers by n inclusions in each layer as a function of the size of one individual inclusion r. Each fig. matches one value n, left to right and top to bottom n = 2,3,5,10, each graph in fig. matches one value N, plots from left to right match N = 2,3,5,10,50,100.

For this case, numerical simulations were also performed, graphs $P_N(r)$ for simulation results and analytical solution are shown in Fig.3 for N = 2,3,5 and 10.

Graphs from left to right – from straight to more curved correspond to N = 2,3,5,10, dots (and thin connecting lines added for clarity) show the results of numerical simulation, lines – analytical solutions $P_N(r)$ subject to appropriate N. As can be seen, the simulation results agree very well with the analytical solution.

4. General case, probability of conduction.

For n>1 the probability of occurrence of a through conductive inclusion obtained by numericalsimulation.

Simulation carried out for the number of layers N = 2,3,5,10,50,100, however, because nature of change since N same for all N to save space in Fig. 4 will only show graphs for N = 2,5,10,100. Each graph set in Fig. 4 corresponds to one value of the number of layers N, each graph probability $P(r)$ from the size of an individual inclusion in the figure – to a certain value of the number of inclusions in the layer n.

The points represent the results of numerical simulations, connected by thin lines for convenience. Also in each figure, the solid curve shows the analytical solution for a given N for $n = 1$. As mentioned above, the results of numerical simulation for $n = 1$ coincide with the analytical solution.

General view of graphs $P(r)$, of course, the same for all N,n is a monotonically increasing function from 0 at $r = 0$ up to one at r = 0,5, when a single inclusion occupies half of the layer, the graphs are shown up to r = 0,6. Graphs for n>1 have an S-shape,

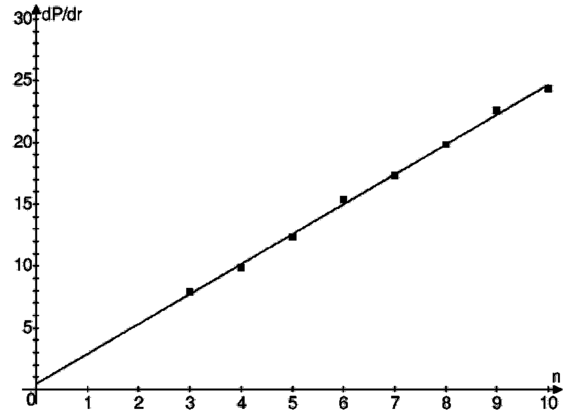

Fig. 6 Slope of the linear approximation of the region of rapid growth of probability $P(r)$ for various n

with a slow rise at the beginning, a fast rise section and saturation, the only exception is the case $N = 2$ where the initial segment of slow growth is not visible. The region of rapid growth is approximately linear.

On graphs for $n = 1$ there is no saturating section. For this case, an analytical solution was obtained, and really, the obtained solution has no saturation part.

It can be seen that the slope of the fast growth area, the growth rate, increases with increasing n, the graph approaches the shape of a step. Meaning of r, at which there is a stepwise jump $P(r)$ from 0 to 1 it is natural to call "percolation threshold".

Graphs move to the right when N growes, the length of the initial section of slow growth increases, the graphs approach the form of a step.

Dependence of the graph shape on N is more convenient to observe in the figures, where each pic. corresponds to a certain value n, and each graph in fig. – value N. Such graphs are shown in Fig. 5

Graphs for $n = 1$ are given above in the analytical solution section. Shown here are graphs for all studied $N = 2,3,5,10,50,100$, and not just those shown in fig. 2.1. It can be seen that with an increase in the number n inclusions in the layer graphics are pressed to the left – an increase in the probability from 0 to 1 occurs with an ever smaller size of a single inclusion r, also increases the growth rate – the angle of slope of the site of rapid growth.

Note that for large n in the area of rapid growth, the graphs are almost parallel to each other, i.e. the slope of the fast growth

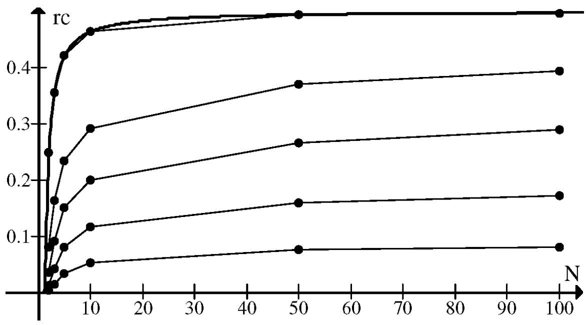

Fig. 7 Percolation threshold $r_c(N)$ for $n = 1,2,3,5,10$ (top down)

area is a function of n and almost independent of the number of layers N.

Values of the slope of the area of rapid growth for various n at $N = 10$ (one of the median values) are given in Fig. 6

Values of the angular coefficient lie quite accurately on a straight line.

As noted above, with increasing n,N graphs approach step shape and value r, at which the jump occurs, it is natural to call the "percolation threshold". Since the graphs still have a certain finite slope angle, we will take as the threshold value $r = r_c$, at which the probability of occurrence of a through conductive inclusion is equal to $P\left(r_c\right)=\frac{1}{2}$. Let us extend this definition to non-stepped graphs.

For case $n = 1$ the only one inclusion in the layer the value of the percolation threshold determined in this way r_c for different values of the number of layers N can be found analytically. It is shown above that when $n = 1$ $P_N(r)=(2r)^{N-1}$. So the value r, at which $P(r)=\frac{1}{2}$, equals

$$r_c = \frac{1}{2}\left(\frac{1}{2}\right)^{\frac{1}{N-1}}$$

In Fig. 7 the percolation threshold values r_c are given as a function of the number of layers N for different number of inclusions in the layer n.

Dots show values obtained from dependencies $P(r)$ found in the simulation and shown above, the points are connected by thin lines for clarity. For the case $n = 1$ the solid line shows the analytical solution. As you can see, the points obtained numerically coincide with the analytical solution.

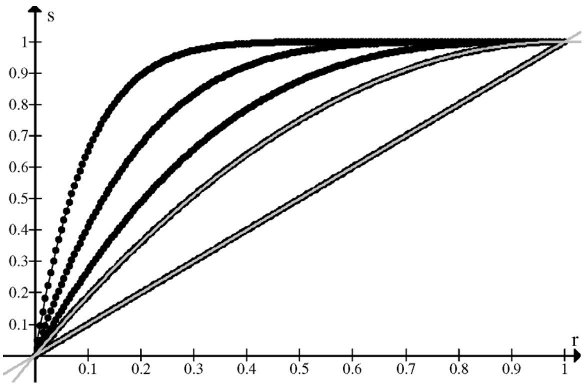

Fig. 8 Average filling of the layer with the conductive phase $s(r)$, graphs from bottom to top match $n = 1,2,3,5,10$

It is interesting to note that at large N percolation threshold values for consecutive n are approximately the same distance apart. Sequential values $n = 1,2,3,5,10$ relate to each other, the following to the previous, as $1:2:1,5:1\frac{2}{3}:2$, i.e. ratios are close in magnitude. Perhaps the values r_c depends on n as a logarithmic function.

Percolation threshold value for $n = 1$ for large N tends to 0,5, the value of the inclusion size, at which the through conductive inclusion is guaranteed, two sectors of size greater than half a full turn necessarily intersect in every two adjacent layers. This effect is typical for graphs $P(r)$, close to the threshold – instantly increasing from 0 to 1 near some r, then r at $P=\frac{1}{2}$ close to r at $P\rightarrow 1$, for flatter plots the values of the percolation threshold will differ from the values r guaranteed conductive inclusion.

5. Filling.

Although the control parameters for the formation of the conductive phase in the layer are n and r, we can assume that the value of the probability of formation of a conductive inclusion is primarily affected by the total filling of the layer – the fraction of the layer filled with the conductive phase, which is a function of n,r. Since the distribution of inclusions in the layer, and hence the degree of their intersection, is a random variable, then the filling will randomly vary from layer to layer, so we will use the implementation-average filling of the layer $s(n,r)$.

At $n = 1$ the filling of the layer is the same as the size of the individual inclusion, $s(1,r) = r$.

At $n = 2$ find the average filling as an average over all possible positions of the second inclusion relative to the first one. At $r<0,5$

$$s = \int_0^r (r+x)dx + \int_r^{1-r} 2rdx + \int_{1-r}^1 r + (1-x)dx$$

where x – angle of the left radius of the second inclusion relative to the left radius of the first one.

$$s = r(2-r)$$

At $r>0,5$ the result is the same.

For $n = 1$, $n = 2$ and larger n average filling $s(r)$ for different r found in simulation, Fig. 8.

The dots show the simulation results, the gray lines show the solutions found above analytically. As can be seen, for those cases for which an analytical solution has been found, they completely coincide with the simulation results.

Plot graphs of the probability of formation of a conductive inclusion from filling s at various n. Graphs obtained for $N = 2,3,5,10,50,100$, as in the section above, to save space, we present graphs for $N = 2,5,10,100$ Fig. 9

First of all, it should be noted that under no N, neither for small nor for large graphs merge into one, i.e. the probability of formation of a conducting inclusion depends not only on the total effect n and r – filling, but also from the control parameters separately. Cases "one big inclusion" – $n = 1$ or small n – and "many small inclusions" with the same filling from the point of view of the appearance of a conductive inclusion are significantly different.

Next, if the graphs $P(r)$ with increase n rose monotonously - each next one passed above the previous one for all r, then already at $N = 2$ graph from filling for $n = 1$ at some s outrunes the rest and further, with an increase N this effect is increased.

Case $n = 1$ as mentioned above, special, in which the filling is equal to the size of the conductive inclusion in the layer, there is no intersection of several inclusions, so there is no decrease in filling compared to $n \cdot r$ due to crossing.

The third thing to note is that the density of points in the graphs in their visible

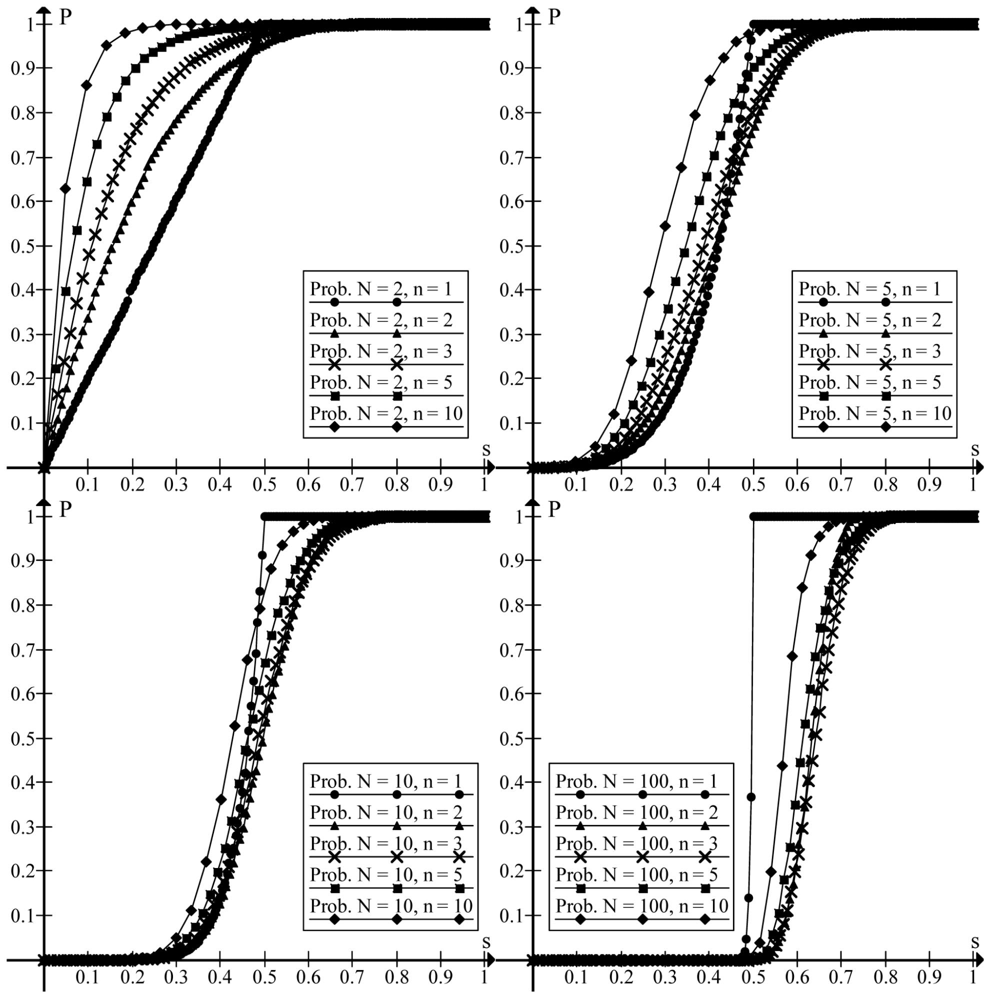

Fig. 9 Probability $P(s)$ formation of a through conductive inclusion in the sample of N layers by n inclusions in each layer as a function of layer filling s. Each fig. matches one value N, left to right and top to bottom $N = 2,5,10,100$, each graph in fig. matches one value n, graphs for $n = 1,2,3,5,10$.

part is nonuniform – both within the same graph and different for different n, even though they correspond to a uniform set of values r. This effect is associated with an uneven change in filling s with r, see graph $s(r)$ above. Therefore, a significant part of the points with different r appears in the area $s \sim 1$, i.e. are projected to one or almost one point of the graph $P(s)$.

Graph outrunning effect for $n = 1$ of other graphs increases with N, at $N = 10$ overtaking occurs not closer to the end, but approximately in the middle of the rest of the graphs, with $N = 100$ overtaking occurs already for the first points for which $P(s)$ different from zero.

But in addition, for sufficiently large N other graphics begin to change places. At $N = 10$ graphs for $n = 2$ and $n = 3$ almost merge, with $N = 100$ graph for $n = 2$ ahead of graph for $n = 3$.

Let's return to the percolation threshold. Let's build a graph of the filling threshold value s_c – such filling s, at which $P = \frac{1}{2}$. Graphs are given in Fig. 10. For $n = 1$ the graph obviously matches the graph r_c threshold r.

Symbol $\cdot$ shows percolation threshold values for $n = 1$, they match the values r_c, the solid line shows the previously analytically found function $r_c(N)$ at $n = 1$.

For $n>1$ graphs s_c before $N = 100$ arranged from top to bottom in ascending order n, however $N = 50$ values s_c for $n = 2$ and $n = 3$ practically coincide, and at

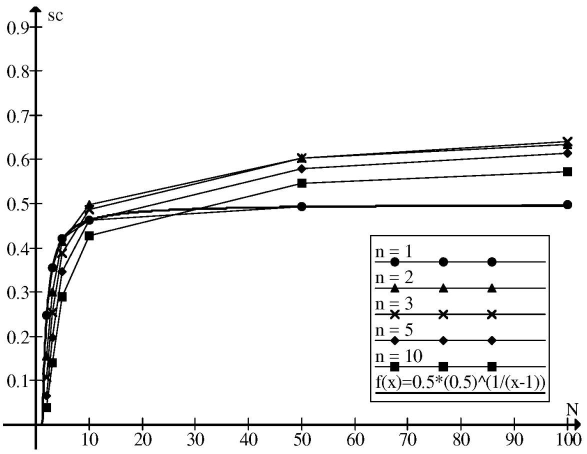

Fig.10 Percolation threshold $s_c(N)$ as a function of the number of layers N for different number of inclusions in the layer $n = 1,2,3,5,10$

$N = 100$ value for $n = 3$ getting bigger, ahead of graph for $n = 2$.

They also behave more complex in relation to the graph for $n = 1$. Values s_c for $n>1$ at small N less s_c for $n = 1$, but for large N get bigger. For achievement $P=\frac{1}{2}$ for large N larger fill values are required than with $n = 1$.

Note that, at least for large $N \geq 10$ graphs run almost in parallel, i.e. behave almost identically up to an additive constant depending on n.

6. The case of "very many very small".

Consider separately the case $n = 100$ inclusions in the layer and $N = 100$ layers, i.e. analogue for the system under consideration of the case of a large number of small conducting inclusions per unit volume of conventional volumetric percolation problems.

Simulation for this case gives a very fast, "threshold" increase $P(r)$ from 0 to 1 on the interval 0,006...0,008, i.e. at very small r. The graph of this section is shown in Fig.11, for clarity, the graph is built for r from 0 to 0,01

The graph for the same case from filling is shown in Fig. 12, here the interval along the horizontal axis is normal, from 0 to 1.

Threshold increase $P(s)$ occurs near fill value $s = 0,5$.

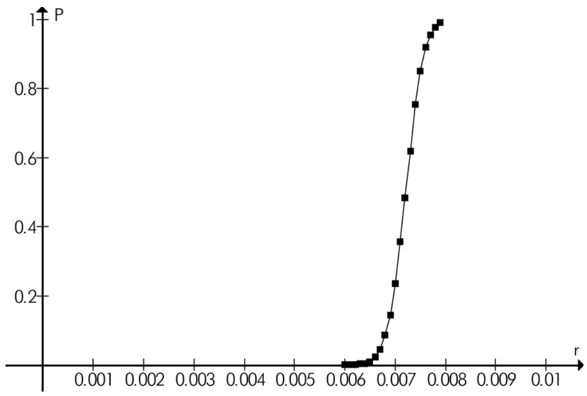

Fig. 11 Section of the threshold increase in probability $P(r)$ formation of a through conductive inclusion as a function of the size of an individual inclusion r for case $n = 100$, $N = 100$

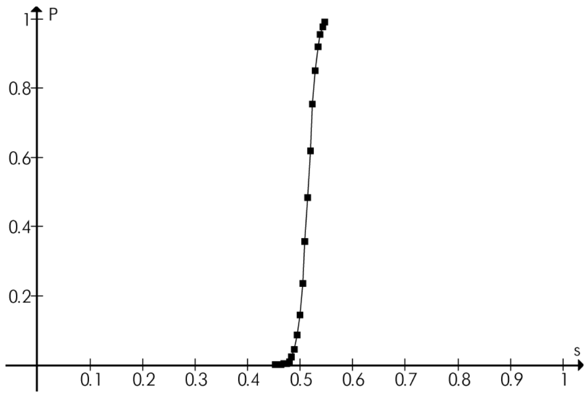

Fig. 12 Section of the threshold increase in probability $P(s)$ formation of a through conductive inclusion as a function of filling s for case $n = 100$, $N = 100$

Conclusions

1. An expression for the probability $P(r)$ forming a through conductive inclusion is obtained for the case $n = 1$ inclusions in the layer analytically: $P_N(r)=(2r)^{N-1}$ for $0 \leq r \leq 0,5$. For $r>0,5$ $P_N(r)=1$. The simulation result coincides with the analytically obtained result, fig.3.

2. For $n>1$ values $P(r)$ obtained by numerical simulation.

a. It is shown that for $n>1$ graphs $P(r)$ have an S-shaped appearance with a slow growth area at the beginning, then a fast, approximately linear growth area and a saturation part. At $n = 1$ there is no saturating section.

b. It is shown that with increasing N and n graphs tend to "threshold" form with almost zero values up to some critical r_c, then instantaneously increasing to one in a very narrow region.

c. It is shown that for large n areas of rapid growth of $P(r)$ for various N almost parallel, i.e. the slope of the fast growing region is a function of n and does not depend on the number of layers N. It is shown that the values dP/dr of the angular coefficient in a given section is linearly related to n, fig. 6.

4. Percolation threshold values r_c obtained for $n = 1...10$, $N = 2...100$, fig. 7.

a. For $n = 1$ expression $r_c(N)$ obtained analytically, $r_c = \frac{1}{2}\left(\frac{1}{2}\right)^{\frac{1}{N-1}}$.

b. It is shown that the values $r_c(N)$ are monotonically increasing functions N and descending of n.

5. Mean values $s(r)$ of conductive phase fill of layer obtained for $n = 1...10$, $r = 0...1$, fig. 8. For $n = 1$, $n = 2$ functions $s(r)$ obtained analytically, at $n = 1$ $s(r)=r$, at $n = 2$ $s(r) = r(2-r)$.

The simuation results coincide with the analitical ones.

6. Dependencies $P(s)$ probabilities of forming a through inclusion obtained as a function of the average filling.

a. It is shown that for various n dependencies $P(s)$ are closer together than dependencies $P(r)$, i.e. the probability of occurrence of a through conductive inclusion depends, first of all, on the filling s, but not n and r separately.

b. However, $P(s)$ for various n do not match. This is due to the fact that with the same filling, but with different n the conductive phase is differently fragmented – with increasing n at one s there is a transition from the case of "one large inclusion" to the case of "many small" with the same total area of the conductive phase.

c. For $P(s)$ a new effect is observed, not observed for $P(r)$ – overtaking by graphs with less n of graphs with large n at some s. Especially noticeable overtaking by graph for $n = 1$ of other graphs. This is due to the fact that the case $n = 1$ special, with $n = 1$ the conductive phase in the layer is not fragmented.

7. Values s_c of percolation threshold received on a scale s, fig. 3.3. For s_c there is also an overtaking effect – graphs for $n>1$ are fast enough to overtake the graph for $n = 1$, because percolation threshold on scale s increases due to phase fragmentation in the layer.

8. Separately, dependencies $P(r)$, $P(s)$ obtained for case $n = 100$, $N = 100$ – an example of a set of parameters typical for percolation problems, "very many very small". Received dependencies $P(r)$, $P(s)$ have a threshold form, according to the scale s – near $s = 0{,}5$, on a scale r – in a very narrow area $r = 0{,}006...0{,}008$, which is typical for percolation problems.

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