ЗАГАЛЬНОНАУКОВІ ПРОБЛЕМИ РОЗВИТКУ СКЛАДОВИХ СИЛ ОБОРОНИ

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THE PROBLEM OF INCREASING THE STRENGTH OF DISPERSE-REINFORCED MATERIALS AS A PROBLEM OF PERCOLATION THEORY

Authors study the continuous percolation problem of clusters consisting of quasilinear and quasi-point elements. The problem is solved by the Monte Carlo method in a cube of 10^6 conventional units of length. Based on the study authors proposed the validation, ground on the percolation theory, for improvement concrete hardening technology known by literary sources. An essential feature of technology improvement is the creation of conditions for the appearance of percolation-type connected regions in dispersion-reinforced heterogeneous materials. These regions consist of accumulations of metal fiber and metal powder, which at critical concentrations cause a sharp increase in concrete strength parameters. The model is considering the possibility of increasing the strength of the material due to mechanical stresses arising at the contact points of concrete with fiber and powder. In addition, article describes the difficulties of the model associated with the hyper-random nature of the data that arise during the study.

Key words: *concrete; dispersed reinforcement; percolation transition; mechanical stress; strengthening.*

Introduction

In the 70s of the twentieth century the elegant concept of disperse reinforcement, as is known, was widely used in the technology of concrete production. Studies of fiber-reinforced concrete have shown that this idea has introduced a number of interesting possibilities into building materials science and solid-state physics as a whole. This researches opened the way for «the development of polyfunctional composite materials that meet many (sometimes contradictory) requirements, and which possess a specific, sometimes unique properties» [1]. One of the research directions was related to the percolation theory that began to form at that time [2-4].

It so happened that building materials science and the theory of percolation did not immediately find common areas of scientific exploration. Meanwhile, the study of the genesis, structure and properties of connected areas in matter, methods of percolation theory, and the subject of the study of building materials has much in common. Both theories use the concept of the hierarchy of a structure of matter and a fractal structure of materials, both of them study of cluster systems, investigate the abrupt change in material properties and other.

Percolation Problems with Quasilinear Elements («Needle» Percolation). Analysis of Recent Research and Publications

Authors of papers [5, 6] was developed model for studying the properties of percolation clusters of elongated elements. The model allows you to search for a threshold concentration of the conducting phase, find contact clusters, calculate fractal dimensions of clusters, determine the length of paths within a cluster, simulate cluster growth dynamics, and more. As the control parameters in the model, the ratio between the length and width of the elements and the maximum allowed angle of deviation of the elements from the axis are used, in particular, the dependence of the percolation threshold on the angular orientation of the elements is obtained for different ratios of the length and width of the elements.

It is shown in the work that the shape of the elongated elements weakly affects the characteristics of the sample: threshold concentrations for rotation ellipsoids and for parallelepipeds converge for the same length to width ratio as it tends to infinity. The authors of [5, 6] believe that the elements of percolation clusters of the model can imitate the structure of spark breakdown: the elements of the model correspond to electron avalanches and streamers, which are ionized sections of the gas. In the work, the effects arising from the multiple simultaneous development of the structural elements of the spark breakdown of gases are taken into account at a qualitative level.

In paper [7] the dependences of the properties of two-phase electrically conductive composite materials with non-stoichiometric titanium compounds on structural parameters were found, and the nature of the effect of additional structuring was determined. According to the authors of [7], the effect is associated with a change in the morphology of the main conductive structure of the material formed by geometrically anisotropic filler particles, which is represented by a system of unidirectional conducting channels and a mesh structure formed by the connection of these channels by conducting bridges of filler particles. This conclusion was drawn from the simulation, in which the shape of the needle particles in the powders of the fillers varied significantly: the ratio of length to width was from 35 to 58.

In [8] was described model for calculating the density of a cluster of carbon fillers in carbon-cement composites. The authors found that if the concentration of carbon fillers slightly exceeds the percolation threshold, then the conductive critical exponent is not universal, and increases with increasing concentration of carbon fillers, and the density of the percolation cluster decreases [8]. For experimental verification of the results, in particular, to determine the actual density of the main (percolation) cluster of fillers, cement composites reinforced with carbon fiber with various concentrations were prepared, and the conductivity current was measured. The results showed that near the percolation threshold, the concentration of carbon fillers is approximately 0.15, which is in good agreement with the simulation results [8].

The electrical conductivity of a carbon fiber reinforced cement composite was studied in [9]. The authors discovered a microstructure associated with the phenomena of electrical percolation: the conduction mechanism was interpreted as being associated with contacting fibers. The changes in electrical conductivity were studied at three different load levels: the threshold value of percolation decreased with increasing load; and also depending on the volume fraction of fibers: at a concentration exceeding the critical, the conductivity of the samples increased by several orders of magnitude. The influence of the volume fraction and length of the fiber on the sensitivity of the measurement of electrical conductivity is shown. The results provide information for the manufacture of conductive and, in fact, intelligent cementitious composites reinforced with carbon fiber [9].

In paper [10] the percolation behavior of nanocomposite systems filled with anisotropic particles with a core-permeable shell structure was studied by the Monte Carlo method. A two-dimensional version of the composite is studied, which is formed taking into account the mutual correlations of the spatial arrangement of particles and using the continuum version of the random sequential adsorption model. The authors of [10] found that the percolation transition in such systems is restrained by the formation of a saturated layer: the percolation cluster arises only if the thickness of the permeable conducting shell exceeds the minimum value, which increases with an increase in the aspect ratio. For orientationally ordered composites, anisotropy of electrical conductivity was observed, which intensified with increasing aspect ratio and filler concentration.

Numerical and analytical studies of the onset of percolation in high-aspect-ratio fiber systems such as nanotube reinforced polymers available in the literature have consistently modeled fibers as penetrable, straight, capped cylinders, also referred to as spherocylinders. In reality, however, fibers of very high-aspect ratio embedded in a polymer do not come into direct physical contact with each other, let alone exhibit any degree of penetrability [11]. Further, embedded fibers of very high-aspect ratio are often actually wavy, rather than straight. In paper [11] authors evaluate the effect of allowing penetration of the model fibers on simulation results by comparing the soft-core and the hard-core approaches to modeling percolation onset. Authors [11] use Monte Carlo simulations to investigate the relationship between percolation threshold and excluded volume for both modeling approaches. The results show that the generally accepted inverse proportionality between percolation threshold and excluded volume holds for both models. In paper demonstrate that the error introduced by allowing the fibers to intersect is non-negligible, and is a function of both aspect ratio and tunneling distance. Thus while the results of both the soft-core model and hard-core assumptions can be matched to select experimental results, the hard-core model is more appropriate for modeling percolation in nanotubes-reinforced composites. The hard-core model can also potentially be used as a tool in calculating the tunneling distance in composite materials, given the fiber morphology and experimentally derived electrical percolation threshold [11].

The onset of electrical percolation in nanotube-reinforced composites is often modeled by considering the geometric percolation of a system of penetrable, straight, rigid, capped cylinders, or spherocylinders, despite the fact that embedded nanotubes are not straight and do not penetrate one another. Authors [12] investigate the effect of fiber waviness on percolation onset. In [12] authors present the results of Monte Carlo simulations studying the effect of waviness on the percolation threshold of randomly oriented fibers in three dimensions. The excluded volumes of fibers were found numerically, and relationships between these and percolation thresholds for two different fiber morphologies were found. Results paper [12] show that for high- aspect-ratio fibers, the generally accepted inverse proportionality between percolation threshold and excluded volume holds, independent of fiber waviness. This suggests that, given an expression for excluded volume, an analytical solution can be derived to identify the percolation threshold of a system of high-aspect-ratio fibers, including nanotube-reinforced composites. Further, in [12] researchers show that for high aspect ratios, the percolation threshold of the wavy fiber networks is directly proportional to the analytical straight fiber solution and that the constant of proportionality is a function of the nanotube waviness only. Thus the onset of percolation can be adequately modeled by applying a factor based on fiber geometry to the analytical straight fiber solution.

Computer experiments to study the structure and properties of ferroceramics were described in [13]. In papers particular attention is paid to the formation of macroscopic connectivity for individual elements of the microstructure and the development of brittle cracks. In addition, the authors investigated the similarity between percolation transitions and the processes of molding, sintering and fracture in technological processes for producing ferroceramics. Based on the idea of the percolation nature of these processes, the articles formulate the concept of the formation of the microstructure of ferroceramics as a sequence of geometric phase transitions, which allowed us to simulate the effect of various microstructural factors on the fracture parameters.

This approach allowed the authors [13] to create computer programs describing real technological processes for producing ferroceramics, in particular, to simulate the processes of crack formation by percolation clusters with linear elements that simulate the sections of cracks.

An analysis of computer experiments showed that if the change in the traditional characteristics of ferroceramics used to assess the degree of completion of technological processes (density, porosity, etc.) is monotonous, then percolation characteristics (average size of small clusters, probability of belonging to a connecting cluster, etc.) have abnormal behavior. Based on this, an assumption was made and analyzed that during geometric phase transitions in real ferroceramics anomalous behavior of such physical characteristics as shear modulus, electrical conductivity and others is possible [13, 14].

In [15] the percolation threshold of hard prolate ellipsoids of revolution dispersed in a continuum is obtained as a function of the aspect ratio. First random close packing of ellipsoids is produced by a dropping-and-shaking protocol. Two ellipsoids are regarded as connected when they come sufficiently close. Then a given fraction of ellipsoids selected randomly is removed and percolation of remaining ellipsoids is investigated as the fraction of remaining ellipsoids is varied. It is shown that the critical volume fraction of the colored ellipsoids is a decreasing function of the aspect ratio and that the aspect ratio dependence is well fitted by the inverse of the interaction range determined by the surface area and the radius of gyration of the ellipsoid surface [15].

Authors [16] present an in-depth analysis of the geometrical percolation behavior in the continuum of random assemblies of hard oblate ellipsoids of revolution. Simulations were carried out by considering a broad range of aspect ratios, from spheres up to platelike objects with aspect-ratio equal 100, and with various limiting two-particle interaction distances, from 0,05 times the major axis up to 4,0 times the major axis. Paper [16] confirm the widely reported trend of a consistent lowering of the hard particle critical volume fraction with increase of the aspect ratio. Moreover, by assimilating the limiting interaction distance to a shell of constant thickness surrounding the ellipsoids, we propose a simple relation based on the total excluded volume of these objects which allows us to estimate the critical concentration from a quantity that is quasi-invariant over a large spectrum of limiting interaction distances. Excluded volume and volume quantities are derived explicitly.

For further progress of the “needle” percolation, the 3D-percolation problem with a mixture of two types of elements – lines and dots is formulated and study; at the same time, for study mechanism of the original technology of concrete hardening, the percolation model of fiber reinforced concrete strengthening is proposed.

Formulation of Goals

The goals of research are to create a percolation model of the phenomenon of hardening, and to determine the range of values parameters of the material, which must ensure increased strength.

Research Material.
Percolating Model of Fiber Reinforced Concrete Strengthening

In [17] the original technology of obtaining steel fiber reinforced concrete with high tensile strength is described. The authors of [17] found that in the developed by them concrete a steel fiber is surrounded by a thin layer, approximately 5÷10 microns, the strength of which is about 2,24 times bigger than the strength of concrete. In order to increase the surface area of steel interacting with concrete, the authors of [17] have changed the ratio between the length, and diameter of the fiber used, and an iron powder was introduced in the cement paste too. Testing of the samples showed that their tensile strength can be 4÷4,5 times higher than the strength of the concrete matrix [17].

A significant feature of the structure of dispersion-reinforced heterogeneous materials is the presence of formed (as a rule, in stochastic processes) fiber and powder clusters. At critical concentrations, these clusters form a connected region of percolation type, causing a structural phase transition. Therefore, they abruptly change the properties of the sample.

In the model, which we proposed, investigated the percolation problem with quasi-point and quasi-linear cluster elements firstly formulated by us for investigate in computer experiments the situations like one described in [17].

The problem is solved by the Monte Carlo method in a cube with a size of 10^6 conventional units of length. The elements that form a model metal cluster are created in a cube using an algorithm that uses a random number generator (RNG) with a uniform distribution. In each model experiment, the fiber has a fixed length: three, five, or seven arbitrary units. Its position is determined by the RNG: it sets the coordinate of its beginning, and then selects from the set (0, ±30°, ±60°, ±90°) the angle of rotation relative to the coordinate axes. Single fibers are considered to be connected if they have a common point or the distance between them does not exceed some specified one. This distance plays the role of a control parameter in the model, as does the length of the fiber. Another parameter of the model is the powder particle diameter. The diameter in each model experiment has a fixed value: one, two, or three arbitrary units of length. The conditions for the integration of quasi-point elements between themselves and with the fiber are determined similarly.

The model considers two factors that can lead to an increase in concrete strength. Firstly, these are small and percolation clusters of fiber and powder, providing dispersed reinforcement. The second hardening factor is the mechanical stresses that can occur during the compression of metal clusters with hardened concrete [18-20].

In [18] it was theoretically study occurrence of mechanical stresses depending on the shape of inclusions. Author [18] shown that quasi-point inclusions create mechanical stresses σ, which decrease with distance as $\sigma \sim r^{-3}$. At concentrations of fiber and powder, sufficient for the existence of a metal percolation cluster in concrete, the mechanical stresses in the material decrease much more slowly with distance. They can be approximated by the following law $\sigma \sim r^{-1}$, and is due to a structural phase transition. A number of parameters change abruptly in the material [4], in particular, a dedicated direction arises [4, 21], and a percolation cluster creates slowly decreasing mechanical stress fields in the material. In their configuration, they resemble fields of quasi-linear defects [18, 22]. A typical fragment of the configuration of the stress field in concrete (based on model experiments) is shown in the Fig.1.

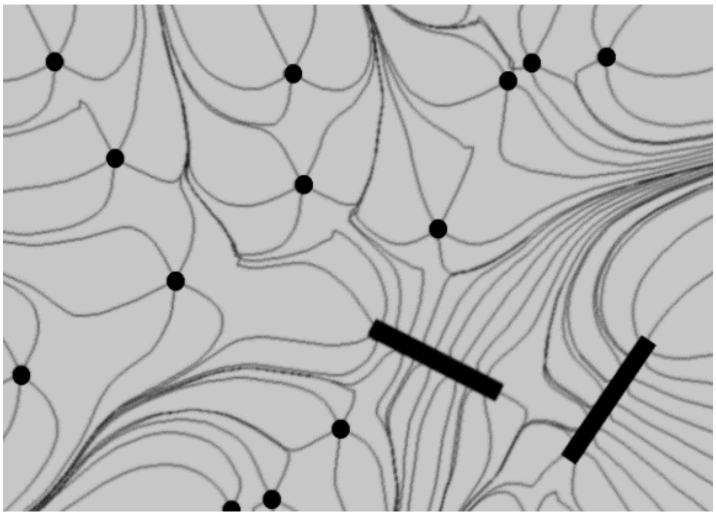

Fig. 1. A fragment of the mechanical stress field, which created by the metallic clusters in the model experiment

The dependences of the percolation threshold and the fractal dimension of a percolation cluster on the concentration of the filler and fiber and powder fractions were studied in our model experiments. At that the percentage of these elements was controlled. To verify the results, we used the percolation threshold for a cluster consisting only of powder, equal approximately to 18% [4].

The simulations revealed an unanticipated subtlety. According to the results of model experiments, it can be seen that the magnitude of the percolation threshold P_c and the fractal dimension D of the cluster consisting of both components in single-type experiments vary in too wide limits, for example, $D = 1{,}41 \div 1{,}71$ and $P_c = 0{,}09 \div 0{,}23$. We deliberately increased the number of model experiments to five thousand, but the scatter of results could not be reduced. May be possible to get closer to the explanation of this phenomenon by the idea of so-called hyper-random variables [23]. They arise in the study when it is impossible to ensure the statistical stability of the phenomenon. Essential for the situation in question is that «the hyper-random estimates in the general case are not consistent, i.e. with an increase of the sample size, their error does not tend to zero» [23]. At the same time, each of the results for the given values of the control parameters was obtained with an error standard for such problems, approximately about 12 percent.

An analysis of the results showed that within the specified conditions the dependences of these characteristics on the parameters of the problem (fiber lengths and clustering conditions) are non-monotonic. For model clusters of fiber and powder, the following laws were obtained, similar to [1, 21, 24]:

– for long fibers, an increase in the maximum deflection angle leads to a decrease in the fractal dimension of the percolation cluster, for small lengths – its growth is observed;

– for large angles at a fixed value of the maximum angle, the value of the percolation threshold increases with increasing fiber length; for small angles – vice versa;

– at a fixed maximum deviation angle with an increase in the length of the fiber: for large angles, the fractal dimension decreases and the cluster power increases, for small angles – vice versa;

– at a fixed fiber length, with increasing maximum deflection angle, the power of the percolation cluster will increase and the value of the percolation threshold will decrease.

Conclusions

The quality of concrete, which is a matrix composite, is largely determined by the properties of the inclusions and the features of their cluster systems. In addition, they are the source of volumetric deformations: many parameters of the material depend on their composition, shape, volume, size distribution, and others.

The proposed model, which was provoked by experimental study [17], made it possible for the first time to investigate the percolation problem with clusters constructed of quasi-linear and quasi-point elements. Thus, the study of a new problem of percolation theory has been formulated and started, as well as initial data on some parameters and features of the cluster structure of steel inclusions in concrete have been obtained. The hyper-random nature of results of the simulation described in this article as a require further research.

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ПРОБЛЕМА ПІДВИЩЕННЯ МІЦНОСТІ ДИСПЕРСНО-АРМОВАНИХ МАТЕРІАЛІВ ЯК ЗАДАЧА ПЕРКОЛЯЦІЙНОЇ ТЕОРІЇ

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У статті досліджена відома за літературними даними оригінальна технологія підвищення міцності бетону сумішшю сталевого порошку і фібри. Операбельність технології та доступність інгредієнтів, що використовуються, роблять її привабливою при будівництві широкого класу споруд як цивільних, так і спеціального призначення. Істотна особливість технології – створення в дисперсно-армованих гетерогенних матеріалах зв'язних областей перколяційного типу, що складаються з кластерів сталевої фібри і порошку, які при критичній концентрації викликають стрибкоподібну зміну параметрів бетону, зокрема, міцності.

У статті надано докладний огляд стану вивчення, так званої, «голкової» перколяції за останні двадцять років.

Для дослідження структури і властивостей матеріалу, що створений за згаданою технологією, розроблена перколяційна комп'ютерна модель структурного фазового переходу, що зміцнює. У моделі вперше вирішена континуальна перколяційна задача кластерів, що складаються з квазіточечних і квазілінійних елементів. Задача вирішується методом Монте-Карло в кубі розміром 10^6 умовних одиниць довжини. У комп'ютерних експериментах отримані значення перколяційних параметрів кластерів. Аналіз результатів показав, що залежності цих характеристик від параметрів задачі (довжини фібри і умов об'єднання в кластер) мають нелінійний немонотонний характер.

В моделі також розглядається можливість підвищення міцності за рахунок механічних напружень, що зароджуються в місцях контакту бетону з фіброю і порошком. Також обговорюється механізм виникнення механічних напруг, інтенсивність яких визначається їх конфігурацією.

У статті описані труднощі моделі, пов'язані з гіпервипадкових характером величин, що виникають в дослідженні.

Ключові слова: *бетон; дисперсне армування; перколяційний перехід; механічне напруження; зміцнення.*

ПРОБЛЕМА ПОВЫШЕНИЯ ПРОЧНОСТИ ДИСПЕРСНО-АРМИРОВАННЫХ МАТЕРИАЛОВ КАК ЗАДАЧА ПЕРКОЛЯЦИОННОЙ ТЕОРИИ

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В статье исследована известная по литературным данным оригинальная технология повышения прочности бетона смесью стального порошка и фибры. Операбельность технологии и доступность используемых ингредиентов делают ее привлекательной при строительстве широкого класса сооружений как гражданских, так и специального назначения. Существенная особенность технологии – создание в дисперсно-армированных гетерогенных материалах связных областей перколяционного типа, состоящих из кластеров стальной фибры и порошка, которые при критической концентрации вызывают скачкообразное изменение параметров бетона, в частности, прочности.

В статье дан подробный обзор состояния исследований, так называемой, «игольчатой» перколяции за последние двадцать лет.

Для исследования структуры и свойств материалов, созданных по указанной технологии, разработана перколяционная компьютерная модель структурного фазового перехода, повышающего прочность. В модели впервые решена континуальная перколяционные задача кластеров, состоящих из квазиточечных и квазилинейных элементов. Задача решается методом Монте-Карло в кубе размером 10^6 условных единиц длины. В компьютерных экспериментах получены значения перколяционных параметров кластеров. Анализ результатов показал, что зависимости этих характеристик от параметров задачи (длины фибры и условий объединения в кластер) имеют нелинейный немонотонный характер.

В модели рассматривается возможность повышения прочности за счет механических напряжений, которые зарождаются в местах контакта бетона с фиброй и порошком. Также обсуждается механизм возникновения механических напряжений, интенсивность которых определяется их конфигурацией.

В статье описаны трудности модели, связанные с гиперслучайных характером величин, возникающих в исследовании.

Ключевые слова: *бетон; дисперсное армирование; перколяционный переход; механическое напряжение; упрочнение.*