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# Structure Modelling Based on Percolation Theory

**W. Trzaskowski *, D. Myszka**
Department of Metal Forming and Casting, Institute of Manufacturing Technology,
Faculty of Production Engineering, Warsaw University of Technology, ul. Narbutta 85, 02-524 Warsaw, Poland
*Corresponding author. E-mail address: wtrzaskowski23@wp.pl

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## Abstract

The paper discusses the possibility of application of percolation theory to model the structure of materials in a virtual space. The designed models were transferred to real space using modern incremental manufacturing techniques like 3D printing. Studies of model materials of this type based on percolation theory are expected to provide more accurate knowledge of the problem, which is extremely important from the point of view of the properties of most construction materials. Reference of percolation phenomena to materials science is more and more frequently done in the design of various types of composite materials, such as e.g. conductive composites. In this study, the percolation theory has been used to design in microscale an optimum material through model analysis done in macroscale. Since studies of percolation in polycrystalline materials are difficult, and there are also some technical limitations imposed on the evaluation done in a volume of material, this phenomenon is usually examined in a simplified manner, which means that it is reduced only to statistical analysis of potential percolation with determination of its threshold value. To generate a potential structure based on percolation theory, popular computer programmes for solid modelling were used. Real shapes were conferred to the designed models using a widely known technique of 3D printing. It allows the production of parts in ABS material. The subject of the present study combines modern design techniques with modern manufacturing techniques, relating both to the fundamentals of materials science. Today's software tools enable creating more complex solids, while their transfer to reality allows better understanding of dependencies that exist in the structure of materials. The originality of this study consists in the art of creating new construction materials with planned properties. The article offers a new approach to the capabilities of scheduling modern engineering materials with the help of percolation theory.

**Keywords:** Percolation theory, Incremental manufacturing, 3D printing, Design of materials

## 1. Introduction

Percolation phenomenon has been known to scientists for many decades. Originally percolation was used only to describe the process of leakage or filtering of fluid through a network of fine channels [1]. Generally speaking, this theory can be used to explain a number of phenomena such as the spread of disease in a population or fluid flow in porous media. These examples belong to a group of disordered systems with stochastic geometry, where random processes play a significant role. For a full discussion of this phenomenon it is necessary to give a definition of the most important parameters that determine the percolation effect. The basic parameter is the percolation threshold. This is the limit value which, when exceeded, causes a transition from one condition/state to another, to mention as an example the local spread of virus of a contagious disease which, when a given number of infected persons is exceeded, changes into the state of global epidemic [2,3].

The discussion of percolation also includes another term referring to a trajectory that this phenomenon follows in its development. This trajectory is called the percolation path. For example, a system of interconnected individual grains of which a spatial structure is composed forms a percolation path. Obviously, in a structure like this, the percolation occurs in three dimensions, which additionally complicates the assessment and quantitative determination of its degree (Fig. 1) [ 3].

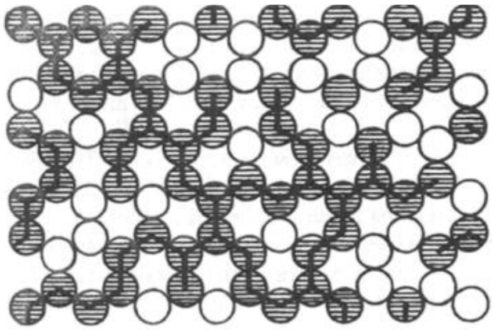

Fig. 1. Example of percolation path for nodes present in a two-dimensional hexagonal grid. Each node is marked as a circle with a radius equal to ½ distance between the nearest neighbouring nodes. Blank circles correspond to the blank nodes, the shaded circles are filled nodes, while clusters of connections are marked with thick lines [4]

The use of percolation phenomena is most common in the fabrication of conductive composites for electronic applications (Fig. 2) or in the concrete permeability test for construction industry.

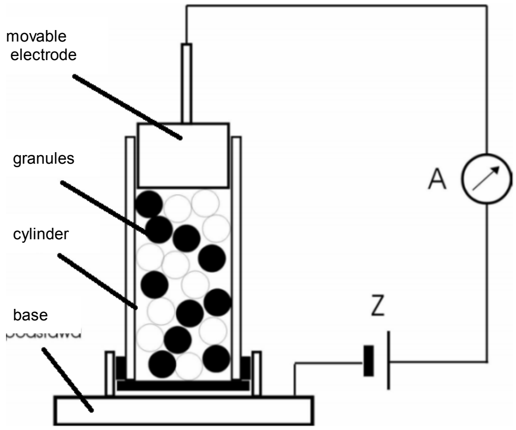


Fig. 2. Example of practical experiment to study the percolation effect in a conductive composite [3]

The percolation phenomenon is known and used in studies of polycrystalline materials. Until now, however, it has not got a precise quantitative method of assessment. The use of this phenomenon is limited only to a descriptive method characterising the observed macro - or microstructure and its morphology in the examined polycrystalline material. Literature gives information on the uniform distribution of the grains of individual phases in a structure, on the grain size, and on the prevailing content of individual phases, or it just describes the shape of the observed particles.

Percolation in crystallography is a phenomenon strongly affecting the mechanical properties of materials. Let us imagine a material with a structure that comprises two phases A and B. These phases can be arranged in two different ways, as shown by the model cross sections in Figure 3. No great knowledge of materials is needed to understand that properties of both these structures will be different. At the beginning, the analysis of such materials should be carried out in a two-dimensional system since any attempt at "spatialisation" will cause considerable difficulties in interpretation (Fig. 4) [ 4,5].

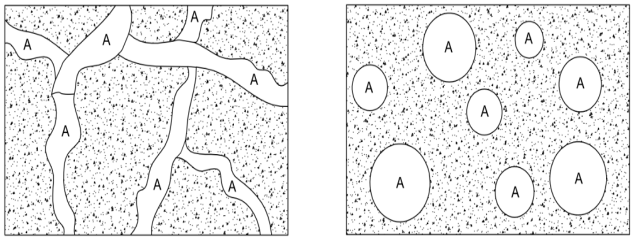

Fig. 3. Percolation of phase A in the structure of model material;
a) percolation occurs – content of phase A – 23.5%,
b) percolation does not occur – content of phase A – 24.1%

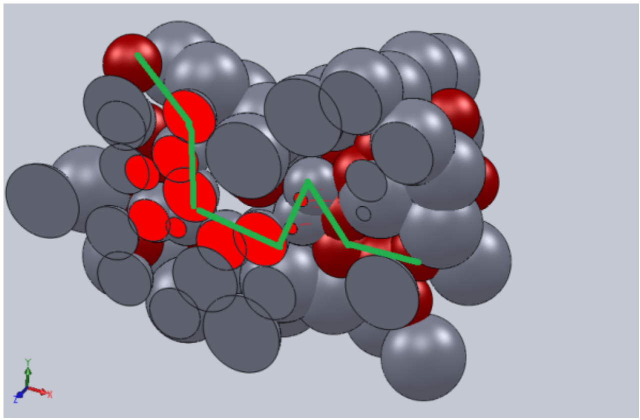

Fig. 4. Percolation path in a three-dimensional model of two-phase material

Knowledge of the problem of percolation in technical sciences is not sufficiently widespread, and therefore the authors of this study have undertaken research works focussed on this particular subject. Some of the results are highlighted in this article.

## 2. Methodology and results

The first step in the programme of studies was to make virtual models based on the phenomenon of percolation. To create such models, a popular software for solid modelling SolidWorks 2010 has been used.

Preliminary models of materials with the preset degree of percolation were generated. The models were a much simplified form of the real structure of the examined phase present in a two-phase metal alloy. Then, using these models, an attempt was made to produce the phenomenon of percolation in alloy structure by designing a series of holes in two planes and transverse partition walls to control this phenomenon. The next step, depending on the needs, included redesigning of the partition walls in such a way as to either provoke the percolation by leaving the holes open or arrest its occurrence by closing the holes in the structure of the material.

Examples of percolation models presented below (Fig. 5) are only a macroscopic representation of the real material, e.g. of the crystal structure in a two-phase alloy.

a) b)

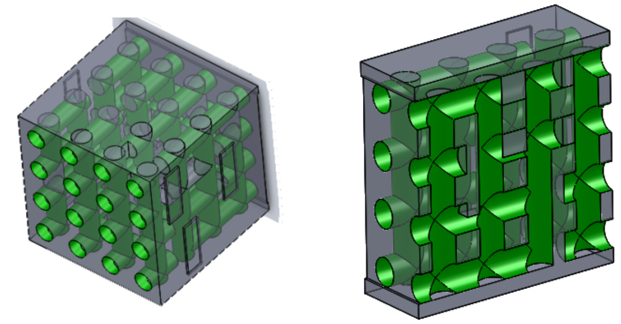

Fig. 5. An example of the simplified model of percolation; a - general 3D view, b - 3D view of the cross-section

Obviously, in the case of the model in question, it should be assumed that the empty spaces (marked in green) belong to one "phase", while the remaining spaces belong to the other phase. The model was designed in such a way as to make the two opposite walls connect the inner spatial network of channels of one "phase". Below there are some images of cross-sections made in the virtual model to show the phenomenon of percolation (Fig. 6). Looking at the cross-sections, a conclusion can be drawn about the presence or absence of percolation in some of the sections. This can be referred to metallographic studies, which illustrate the examined material in planes of the selected sections.

a) b)

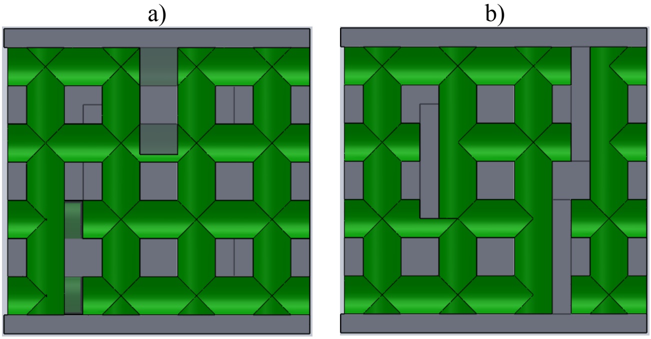

Fig. 6. Examples of cross-sections made in the designed model; a - the first row of holes (percolation occurs in this plane), b - the fourth row of holes (percolation does not occur in this plane)

Due to the complexity of the virtual model, real models were made by the technology of incremental manufacturing, i.e. by the technique of 3D printing. Printing was done using a MAX3D Printer that makes models in the ABS (acrylonitrile-butadiene-styrene) copolymer material. After printing, the models were subjected to a superfinishing treatment with acetone to smooth the outer surfaces. Below there is a picture of the printed model used for studies of the percolation process (Fig. 8).

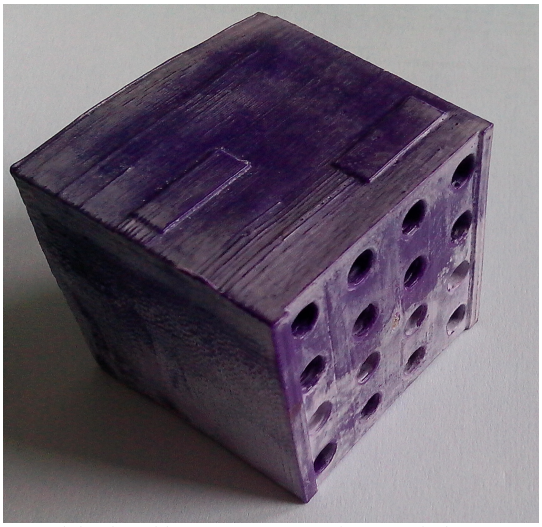

Fig. 8. Model printed in ABS to assess the percolation process

## 3. Summary

The main aim of the studies was to design and build a real, three-dimensional model for the evaluation of percolation effect in engineering materials. On the basis of this study, through the analysis of simplified models, it will be possible in the future to analyse and understand the structure of materials in their internal architecture (phases, skeletons, etc.).

The reference to two-dimensional images, which the metallographic images are, is justified by later reference of models to real materials and structure evaluation done in the entire volume. The data acquired in this way are expected to be useful in the future work when spatial models of the real structural materials are created basing on the two-dimensional images of polished metallographic sections.

So far, in the field of materials research, the phenomenon of percolation has been treated with little interest. The works completed mark only a starting point on the long road leading to more profound studies of relationships that are said to occur between material properties and a complex spatial structure. The research described in this paper is expected to lay the foundations for the implementation of further actions to assess the percolation phenomena in engineering materials.

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