11th IYPT '98

solution to the problem no. 12
presented by the team of Belarus
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Powder conductivity

Measure and explain the conductivity of a mixture of metallic and dielectric powders with various proportions of the two components.

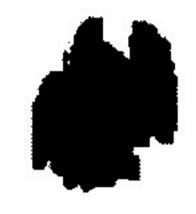
Overview

- Experiments
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1 Experiments

For the solution of the given problem we used powders of the following materials:

- 1. Ironic powder, particles of which have irregular form of 0.03 mm size.
- 2. Sodas, as a dielectric, particles of which are crystals of 0.04 mm size.



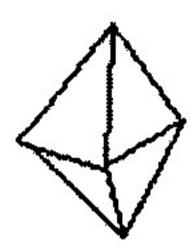


Figure 1: Powder

We chose soda because of the size of its powder particles. They are approximately equal to the size of ironic particles. We determined the size of particles by microscope. While making experiments we noticed, that results depend on many factors, such as way of mixing and pouring powder into the tube. As an example we show the results of experiment when the concentration of ironic powder is about 65%. We define concentration C as the ratio of quantity of the ironic particles to the whole number of particles in the mixture. Afterwards instead of concentration of ironic powder we'll say concentration. It's useless to operate with any kind of errors because of the accidental nature of an investigating process.

For subjective factors influence the experiment, for the solution of that problem we used an experimental device which as far as possible minimises their dependence on the results of the experiments. A mixture of powders was placed into a glass tube of 1 cm diameter under the pressure of 100 g load. Electrodes were slim copper plates. We can find out the resistance of the mixture by applying obtained physical values to the following formula. The results of experiment: C = 65%, $I = 3.0 \,\mu\text{A}$, $R = (7.7; 62; 12; 33) \,\text{M}\Omega$.

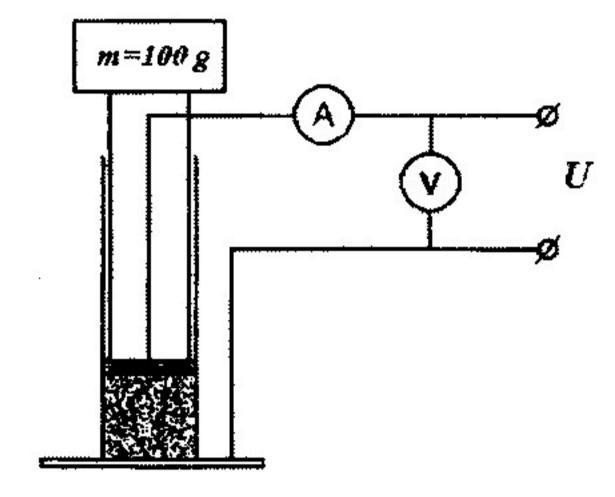


Figure 2: Setup

$$R = \rho \frac{l}{S}$$

$$R = \frac{dl}{dt}$$

First of all we made experiments with pure ironic powder. These experiments proved that resistance of ironic powder depends on electric current, moreover this dependence is non-linear. As a result the OHM LAW doesn't work. We also investigated the powder on the dependence of resistance on the distance between the electrodes. This dependence is also non-linear. In such a case the standard formula for estimation of resistance is inapplicable. Therefore all following series of experiments were made at current 3 mA and distance between electrodes 1 cm. Then we approached the main aim of our investigation: To find relation between the resistance of mixture and concentration. The results of the experiments are shown on the graphs in figure 3.

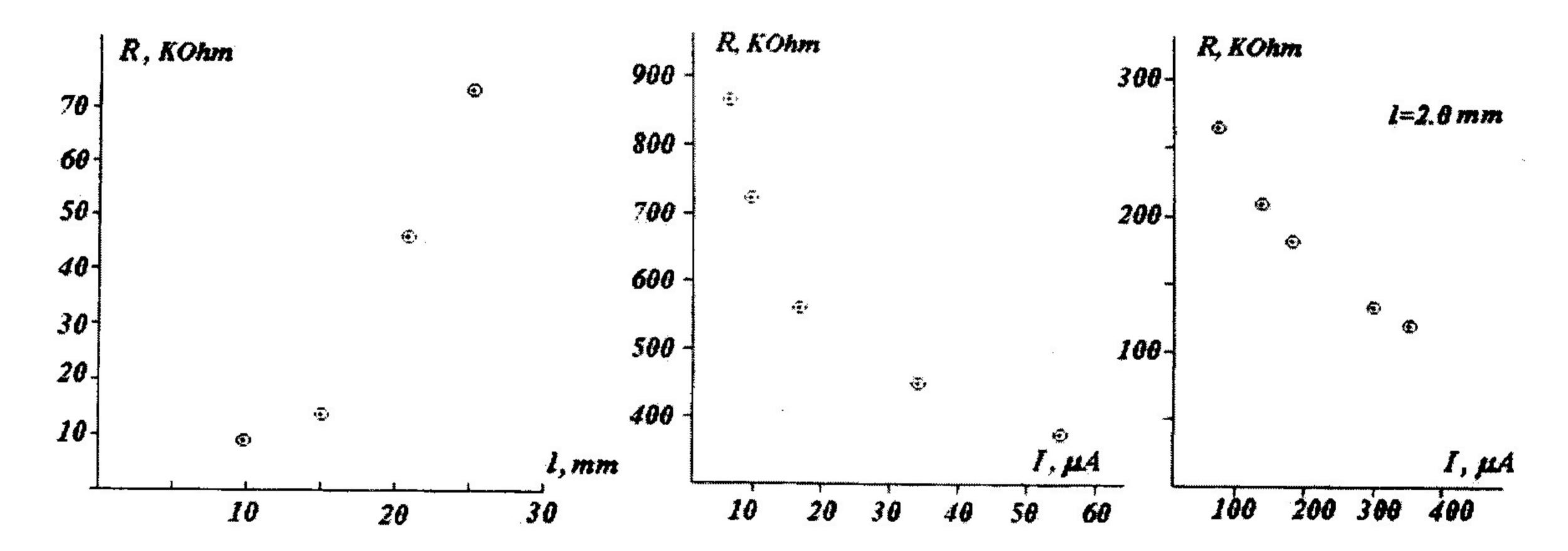


Figure 3: The dependence of resistance on the distance between the electrodes and of the resistance

Current 160 µA

O 012 1 0 1 1 0	F
$l~(\mathrm{mm})$	$R~(\mathrm{k}\Omega)$
10	10.0
15	13.8
20	48.1
25	68.1
30	230
	10 15 20 25

During the experiment we were faced an interesting phenomenon. When dielectric concentration was equal to 55% resistance of the mixture was unusually high, but at the same time it was the finite value. As soon as we increased the concentration of dielectric by 1% the mixture became nonconductive. That is we faced the phenomenon which is in many ways similar to the second-order phase transition. Mixture grade from the conductive to the dielectric state when the concentration of dielectric equals 55%. Let's call it critical concentration. This phase transition, abrupt jump of mixture's conductivity, appeared most interesting and unexpected for our team. That's why we directed our following investigation to explanation of existence of critical concentration and determination of its value.

2 Computer simulation and Percolation theory

In order to solve this problem we resorted to a computer simulation on the basis of MONTE CARLO method. While studying the articles related to our problem we found out that similar phenomena have already been investigated. They're described by percolation theory.

	93				
C(%)	$R (\mathrm{M}\Omega)$				
0	0.08				
5	0.28				
10	0.78				
15	2.14				
20	6.03				
25	12.0				
30	24.7				
36	33.0				
40	38.7				
45	50				
50	100				
55	≥ 200				

Let us place powder particles in the form of a plane layer. That is, any particle contacts 4 closest particles. Each particle may be either metal, or dielectric. Moreover probability of particle being dielectric equals concentration. By imagination we connect the electrodes to the opposite sides of the tube and switch on the mixture into the electric circuit. It's obvious, the current will flow in case if only the one way of contacted with each other conductive particles, which connect electrodes, exists. In the percolation theory it is called a cluster. In such a case percolation appears.

This model is easy for computer simulation. It has the following algorithm: each cell of lattice has random value 0 (dielectric) or 1 (conductor). Then all conductive cells of the first layer connected with the electrode are assigned value 2 (that corresponds to the conductive cells contacted with the electrode). Then reveal the other cells which are connected to the electrode reveal.

We wrote a demonstration program for the plane square lattice. Blue squares correspond to dielectric, grey to metal particles. White squares conform to particles of the connecting cluster. I'd like to remark that the demonstration program shows work of an algorithm of successive approximations only, but not the dynamics of the real physical process.

The principal problem of our computer simulation is to find critical concentration C (let us call C percolation threshold).

In order to obtain a percolation threshold we plotted a graph of ratio successful attempts to the whole number of attempts depending on the size of the lattice. Let's define a successful attempt as an attempt when the current flows through the lattice. While increasing size of the lattice the tendency to increasing graph steepness is easily observed. Namely this jump on the plot conforms to phase transition of conductor-dielectric mixture. That is, we can say our model is correct, since we obtained the experimental effect in a computer simulation. While increasing size of the lattice to infinity range of concentration corresponding to phase transition shrinks to point. For defining a percolation threshold we confine ourselves to the lattice size 250×250 . In order to prove it let us apply to the graph of dependence of probability that cluster grows up to row number 'I' on concentration. While the concentration is above the percolation threshold probability that cluster grows up to $100^{\rm th}$ row practically equals probability that cluster grows up to $200^{\rm th}$ row. Therefore our approximation (limitation of the lattice of 250×250 size) is quite appropriate.

While investigating the regular square lattice we observed the phenomenon of phase transition. We investigated other types of lattices in a similar way: for plane ones: triangular (number of possible

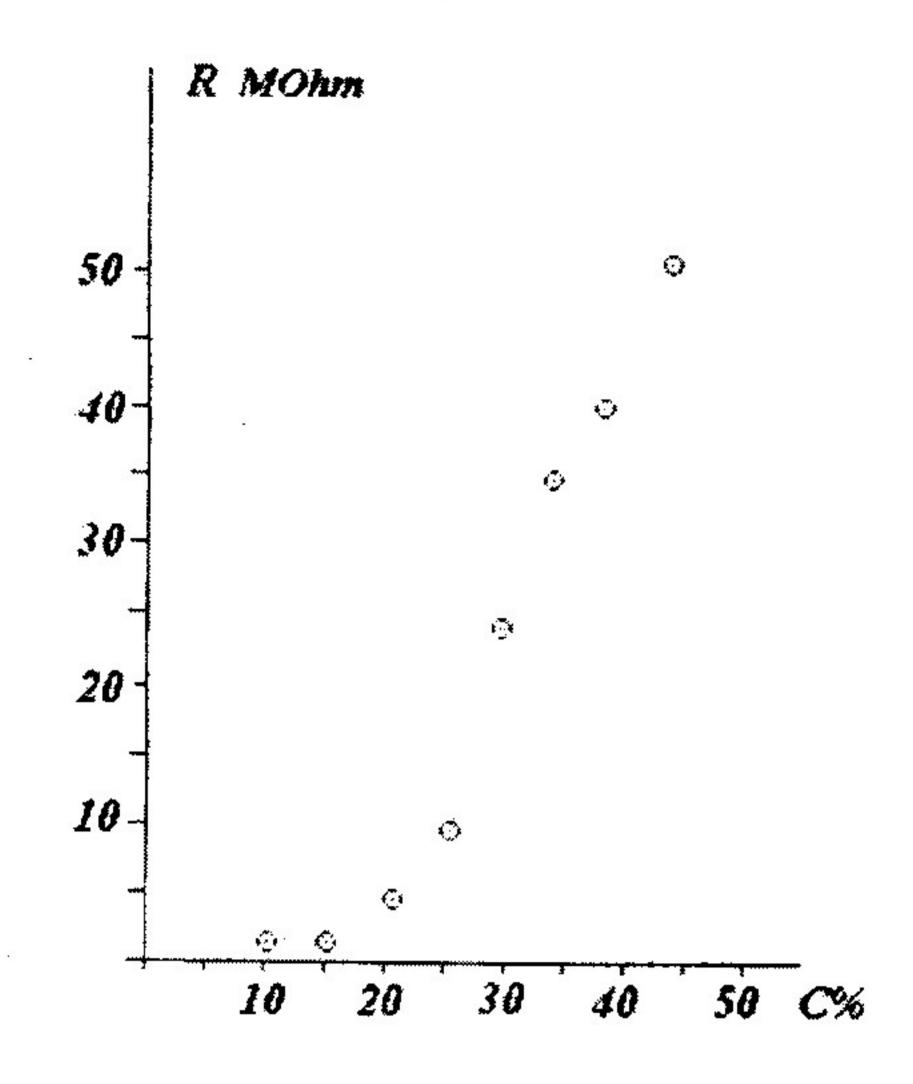


Figure 4: The dependence of resistance on the concentration of dielectric

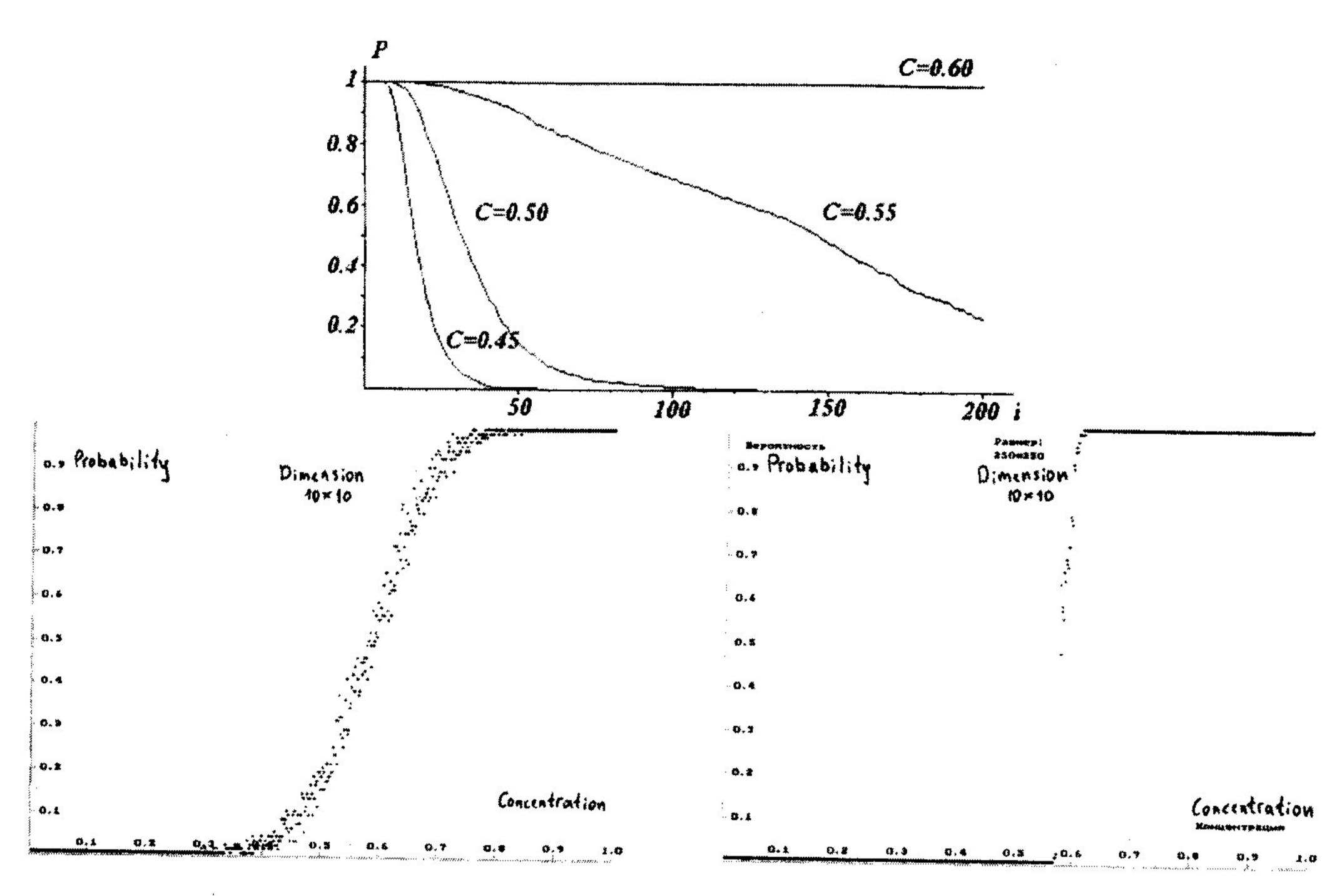


Figure 5: Probability

contacts of one particle, z equals 3), hexagonal (z = 6); and three dimensional lattices namely regular cubic (z = 6), body-centred cubic (z = 8) and hexagonal (z = 12). The phenomenon of phase transition was also observed in other type of lattices also. Their percolation thresholds are shown in the first table.

Let's try to estimate a percolation threshold for an irregular lattice. Let's assume that percolation appears when fraction of the total volume (area) occupied by metal spheres (in plane case circles) exceeds a certain critical value which is independent on the lattice type.

In order to examine such an assumption, we have to calculate parts of the volume occupied by metal spheres at critical concentration for different types of lattices and to compare them with each other.

In order to find out the part of the volume occupied by metal spheres at critical concentration, it is necessary to multiply fill factor f by critical concentration. If the assumption of universality of this volume part at percolation threshold is right, value f multiplied by critical concentration has to be a constant for all types of lattices.

Fill factor, critical concentration and products of these two variables for different types of lattices

are shown in the second table.

Type of lattice	f	$C_{ m cr}$	$fC_{ m cr}$					
Plane								
triangular	0.91	0.50	0.46					
square	0.79	0.59	0.47					
hexagonal	0.61		0.43					
Three dimensional								
regular cubic	0.52	0.31	0.16					
body-centered cubic	0.68		0.16					
hexagonal	0.74		0.16	$C_{\mathcal{C}}$				Ccr
				0.7-	•		0.3-	10.40
Type of lattice	\boldsymbol{Z}	$C_{ m cr}$		0.6-		. •	0.25-	
triangular	3	0.70			······································	······································		
square	4	0.59	Sa.		2 4	6 Z	81.	2 4 6 8 10 12 2
hexagonal	6	0.50				Figure	6. La:	ttice
	0	0.01				1 15410	0. 1 1 1 0 .	
regular cubic	6	0.31						
body-centered cubic		0.24						
hexagonal	12	0.21						

It is clearly seen that both in the group of plane lattices and in the dimensional lattices group the products (of fill factor and critical concentration) almost don't change. Hence the formula is correct for plane lattices to within 5% and for three dimensional lattices to within 3%.

Thus we demonstrated, that percolation appears when the part of the volume occupied by metal spheres is equal to 0.16. This number is almost independent on the type of lattice. Hence it's naturally to suppose that this part of volume remains the same for an irregular lattice, too.

Thus the percolation threshold can be calculated under conditions of a real experiment. In this case the lattice is accidental and the fill factor can be estimated experimentally. The fill factor equals a ratio of mixture density with the air to the mixture density without the air. If we calculate f and substitute it in the formula

$$C_{
m cr.\,exp.} = rac{0.16}{f} = rac{0.16}{0.38} = 0.42$$

we obtain critical concentration for the real lattice. It's equal to 42%.

3 Conclusion

Experiments revealed a phenomenon of phase transition of conductor-dielectric mixture if concentration of iron equals 45%. On the basis of computer simulation we showed that this phenomenon inherent to all kinds of mixtures regardless their structure. We obtained approximate formulas for evaluation of the percolation threshold for both regular and irregular lattices. On the basis of these formulas we calculated the value of percolation threshold. It equals 42%. In this case we have a great agreement between the experimental (45%) and the theoretical (42%) data.