Simulating the formation of conductive networks in composites containing nanotubes

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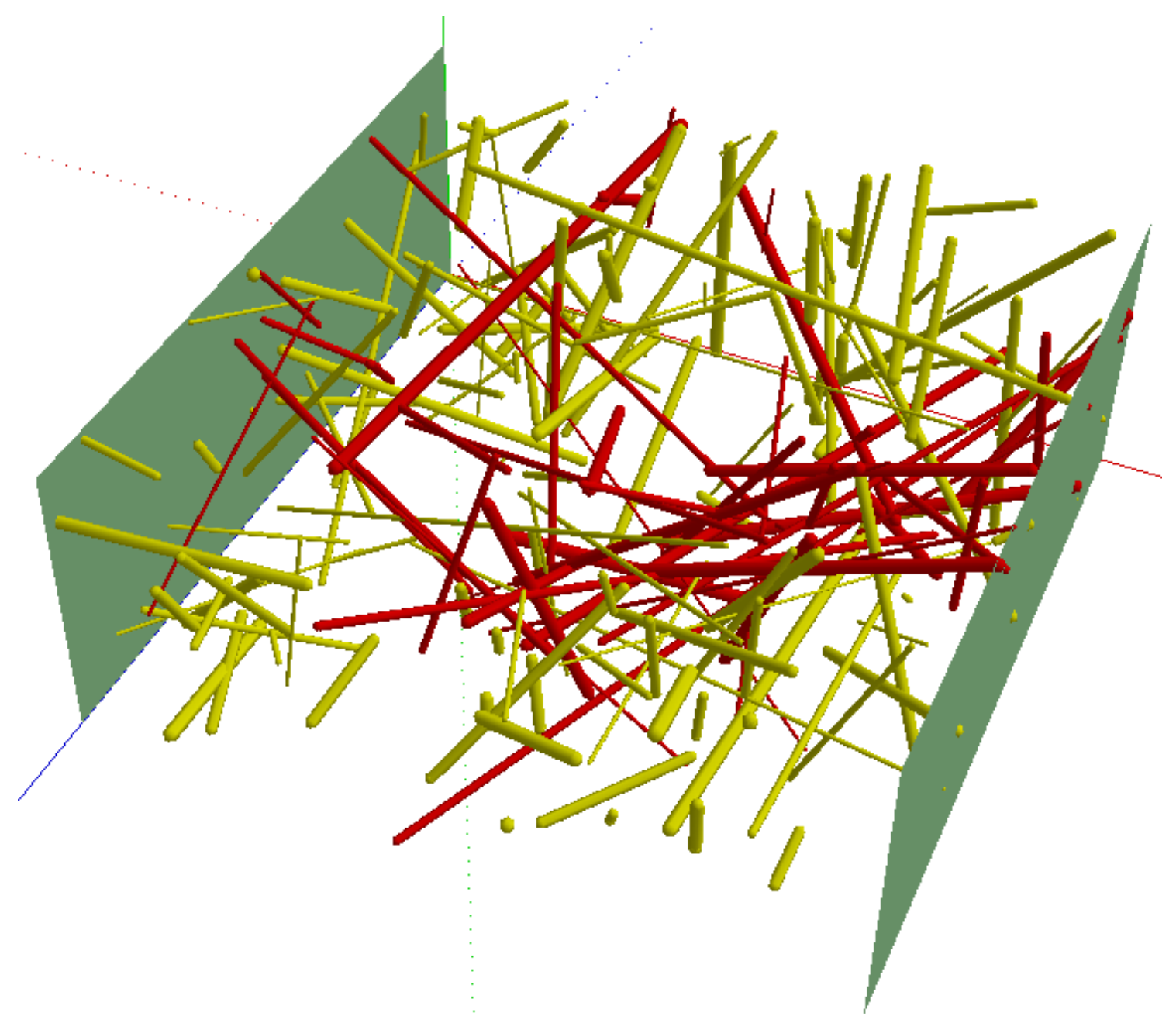
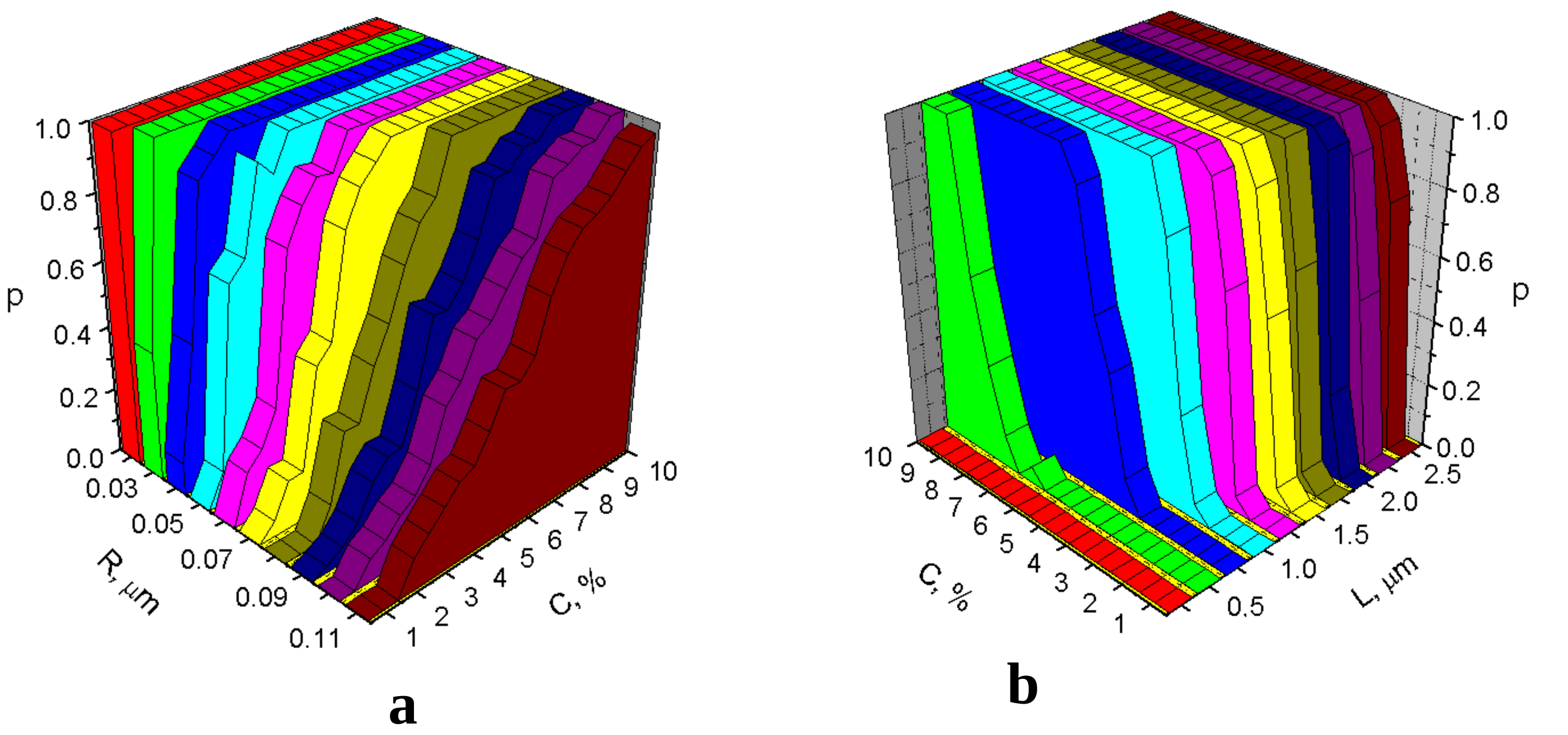
Analysis of percolation phenomenon in the system of straight nanotubes is carried out and an appropriate model of the process proposed. An algorithm for finding the probability of nanotubes percolation is implemented using three-dimensional graphics visualization tools. The effect of geometric size and concentration of the nanotubes on the percolation probability was investigated. Based on the analysis of the dependence of percolation probability on the values of the dispersion angles determining the nanotubes orientation, the basic regularities of the conductive cluster formation under the influence of an electric field are established. The optimal parameters of the nanotube system with field-controlled percolation were determined.



Model of nanotubes system with a highlighted conductive path between two opposite sides of parallelepiped

In the proposed model, the nanotube system is represented as a volume element in the form of a rectangular parallelepiped, in which nanotubes are located chaotically. Nanotubes are considered as hollow cylinders with length L and diameter D to simplify the description of the system. In terms of representation, an individual nanotube is built of three primitive constituent elements: two hemispheres at the ends of the tube, and a cylinder between these hemispheres. The spatial position of each nanotube is determined by the coordinates of two boundary points on the opposite ends of the tube. During the process of the generation of the nanotubes system, the number of elements in this volume is calculated according to the concentration and geometric sizes. Nanotubes can be either isolated or in direct contact with each other.

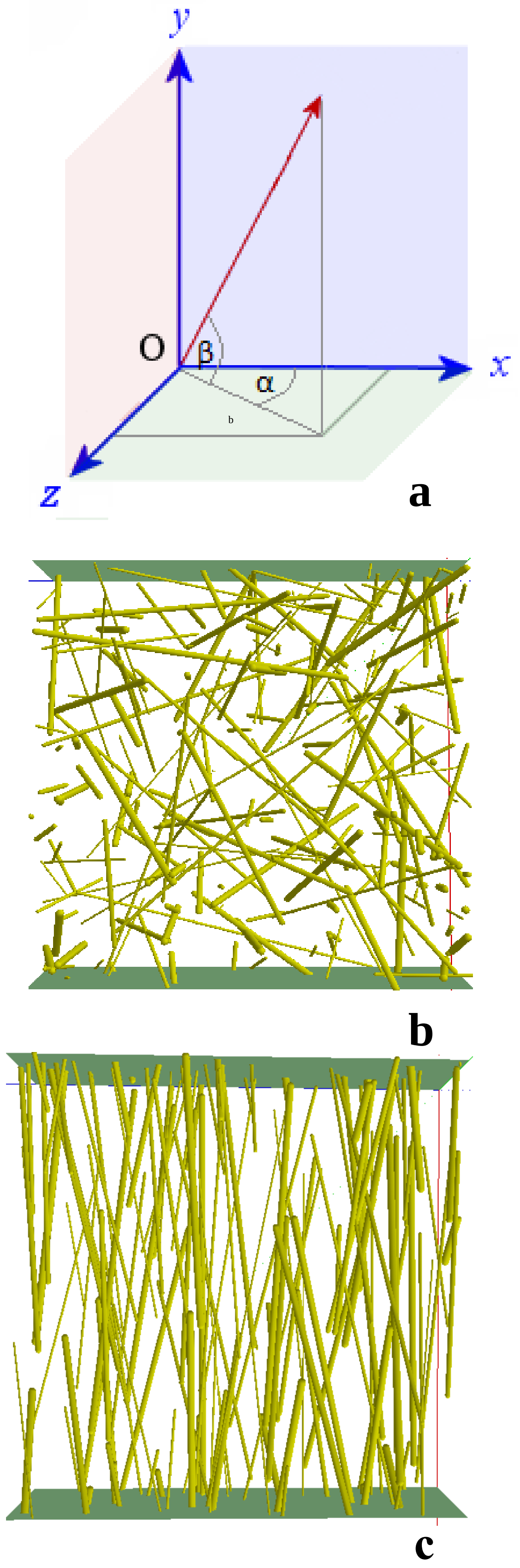


a **b**

Dependence of the percolation probability on the concentration and length of nanotubes (a), on the concentration and radius of nanotubes (b).

Analysis of the obtained dependences indicates a reduction of the percolation threshold due to an increase in the length of nanotubes from 0.5 to 2.5 microns. The minimal concentration of nanotubes that ensure the formation of the conductive cluster decreases from 9 to 2.5%. The increase in the radius of nanotubes from 20 to 110 nm leads to the respective increase in the percolation threshold. It may be related to the decreased number of nanotubes in a given volume and the increase in their diameter for constant volumetric concentrations.

The goal was to study the influence of nanotubes orientation on the percolation probability in the 3D model of the system. For a completely anisotropic system, all nanotubes are oriented along the normal and α = β = 0. The isotropic distribution of nanotubes corresponds to a limit of -90o < α < 90o, -90o < β < 90o. No restrictions on the orientation of nanotubes corresponds to the case, when applied voltage is 0. In the case where α = 0 or β = 0 and an arbitrary dispersion of the other angle, a 2D model of the percolation system can be obtained.

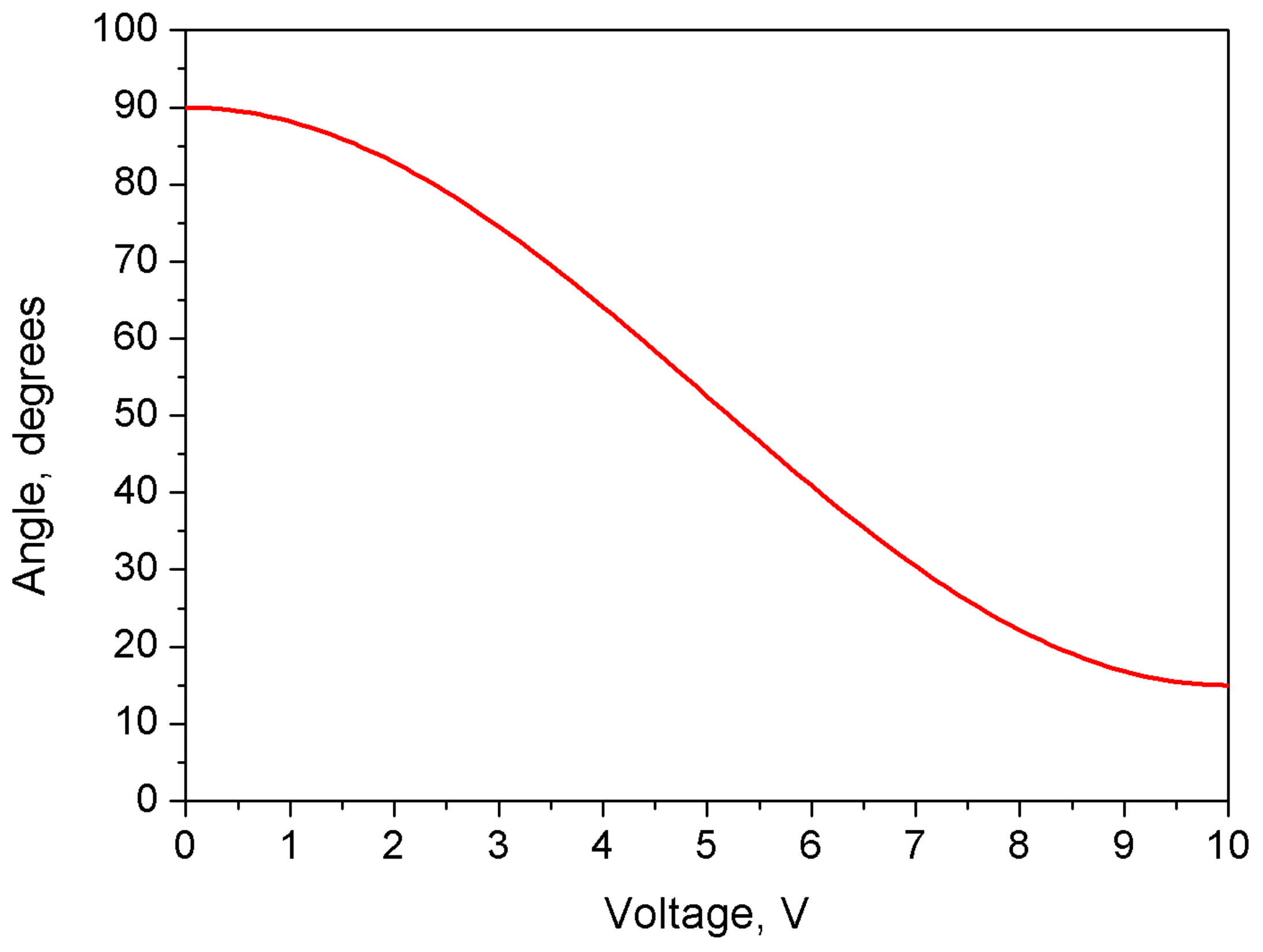


a

b

c

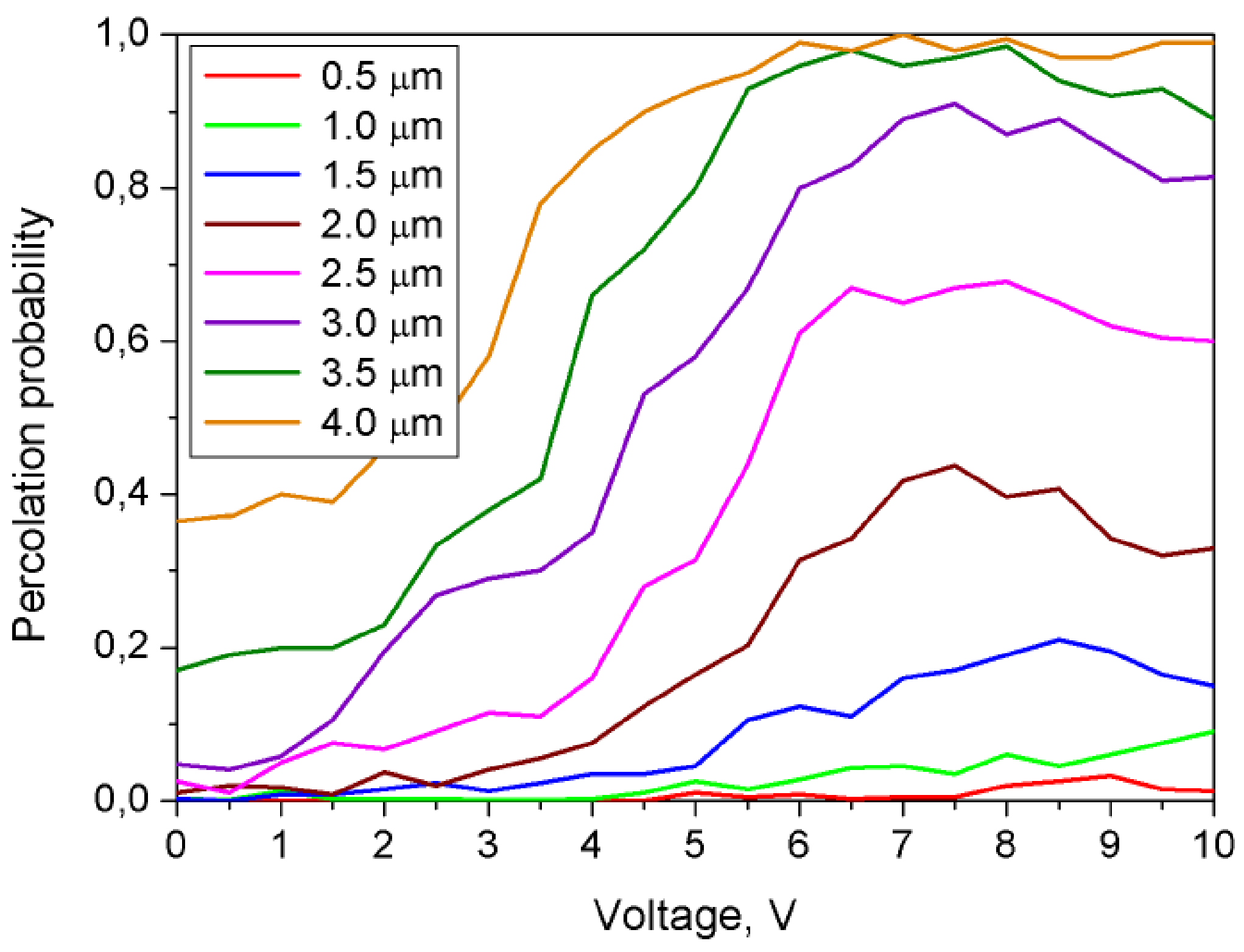
Determination of the nanotube orientation in 3D space (a) and the isotropic (b) and anisotropic (c) nanotubes distribution with the following angular dispersion limitation: -90o < α < 90o, -90o < β < 90o (b); -15o < α < 15o, -15o < β < 15o (c)



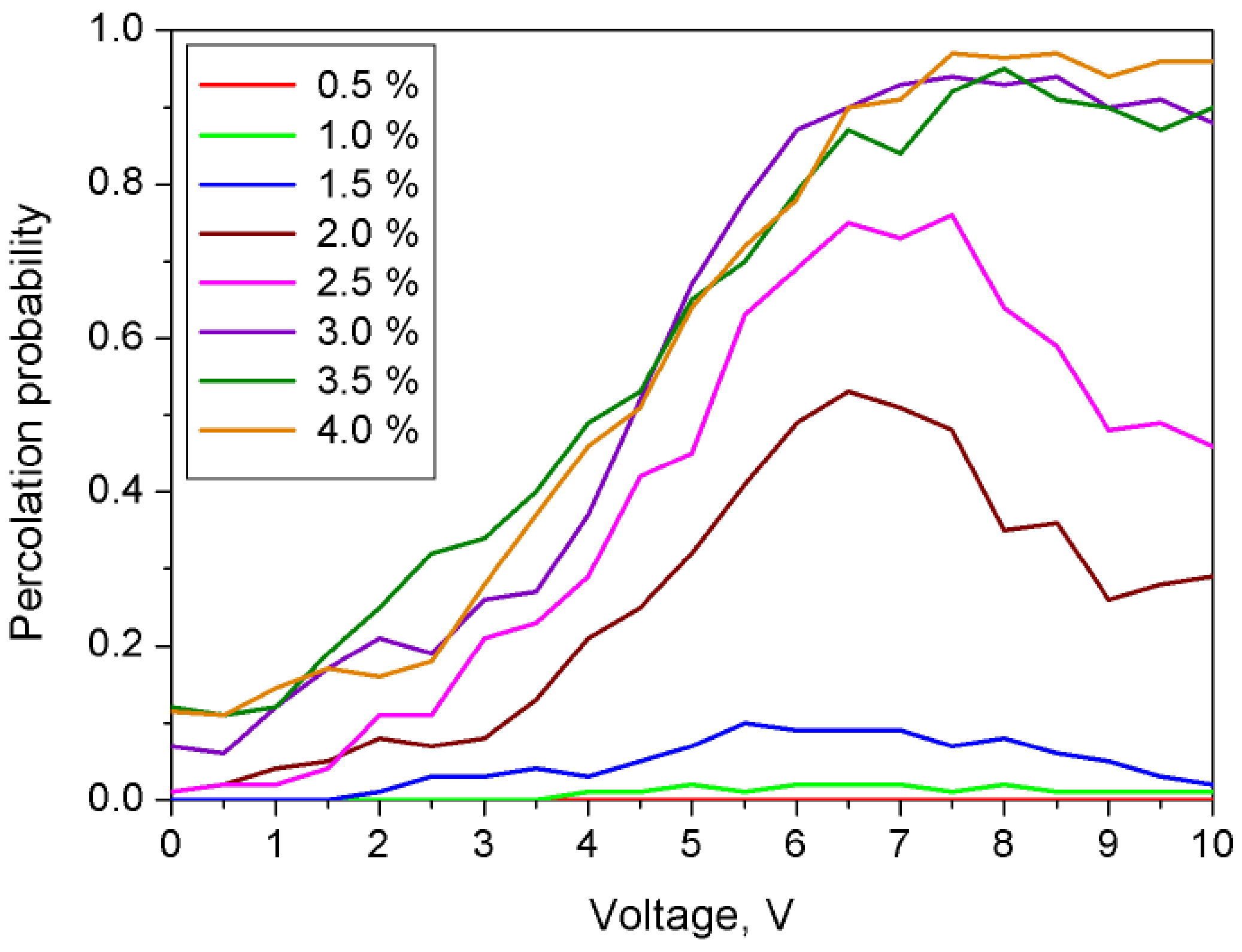
Dependence of the orientation limitation angle of nanotubes on the applied voltage

In order to observe field-controlled percolation in 3D system of straight carbon nanotubes, the dependence of the orientation limitation angle on the applied voltage U was used. Distribution of the nanotubes in disordered system at U = 0 corresponds to the angular dispersion limitation: -90º < α < 90º, -90o < β < 90º. With the increase of the voltage applied to the percolation system, the orientation limitation angle decreases nonlinearly. At U = 10 V nanotubes orientation is limited by about 15o angle. Boundary conditions of the dependence of the orientation limitation angle on the applied voltage are based on experimental results of field-controlled nanocomposite morphology change.

The simulation results show that the percolation probability significantly depends not only on the concentration and geometric sizes of nanotubes but also on their prevailing orientation, which can be controlled by electric field. Fig. 5 shows dependences of the percolation probability on the applied voltage for different nanotubes length. Calculations were performed for the fixed concentration of nanotubes in the composite which was set to 3 %.
If the field is not applied at α = β = 90o the probability of percolation of nanotubes with the length up to 3 nm is close to zero. Increasing the applied voltage leads to the decrease of the orientation limitation angles and, consequently, to the increase of the percolation probability. The obtained results are in good agreement with the data of the studies of the carbon nanotubes system in 2D model. For nanotubes with 3–4 nm length the percolation probability reaches values as high as (0,8–1,0) under the voltage of 5 V. One has to note that at 3 % concentration nanotubes longer than 3 нм can form conductive network even without applied electric field. On the other hand, the efficiency of conductive cluster formation in the system of nanotubes of 0,5–1,5 nm length is low for random orientation. (see Fig. 5). Therefore, optimal length of nanotubes for electrically controlled percolating system is about 3 nm.



Dependences of the percolation probability on the applied voltage for different nanotubes length (nanotubes concentration C equal to 3 %)



Percolation probability as the function of the applied voltage for different nanotubes concentration (nanotubes length *L* = 3 nm)

Based on the analysis of the obtained results, weak dependence of the percolation in the system of straight nanotubes on the distribution anisotropy level was established for the concentration of nanotubes in the 0.5–1.5 % range. Efficient switching of the percolating system to conductive regime under applied voltage above 5 V is granted in nanocomposites with nanotubes loadings of about 3–4 %.