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PROCESS SIMULATION FORMATION OF ISOTROPIC SOLUTION OF CARBON NANOTUBES IN POLYMERS

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The use of carbon nanotubes (CNTs) as additives to the polymer matrix to create new functional composite materials is relevant. The potential for using CNTs as a builder is limited by the difficulties associated with uneven distribution of entangled CNTs during processing and poor interfacial interaction between CNTs and the polymer matrix. The nature of the uneven distribution problem for CNTs is different from that of other fillers such as spherical particles and carbon fibers because CNTs have a high aspect ratio (>1000) and therefore an extremely large surface area. In addition, commercialized CNTs are supplied in highly entangled structures, leading to dispersion difficulties.

The program "NanTu" has been developed to calculate the distribution of CNTs by linear dimensions in a polymer matrix depending on the intensity and duration of mechanical and ultrasonic mixing. The program sets the probability of destruction of CNTs depending on the length of the nanotube. The initial data for the program is the size distribution function of CNTs. The output of the program is the distribution function of CNTs from the processing time. The developed program is used to evaluate the behavior of CNTs in solution during dispersion and optimize the process of preparing composite materials. The obtained results of calculations make it possible to study various mechanisms of CNT destruction.

The algorithm of the program is as follows. At the first stage, the maximum and minimum lengths of nanotubes in solution are set, the length below which the nanotube does not break down, the range of sizes subject to destruction during processing, the discretization step of the nanotube sizes, and the size distribution function of the nanotubes.

At the second stage, the distribution function of nanotubes is calculated for one time interval of solution processing. Successive launches of the program calculate subsequent distribution functions of nanotubes at the following time intervals. The program calculates three types of graphs - the dependence of the mass on the length of nanotubes, the distribution of the probability of destruction and the size distribution of nanotubes (Fig. 1).

Figure shows the results of calculating the distribution of CNTs after three stages of processing 104 identical nanotubes 1 μm long. The resolution probability distribution function has a maximum in the middle of the nanotube. The calculation results show the presence of a maximum in the region of 500 nm, which slowly grows with increasing processing steps. This is due to the successive destruction of the initial nanotubes 1 μm long and the increase in the number of nanotubes of other sizes during processing.

The characteristics of composite materials significantly depend on the type and duration of preparation and processing. The developed software makes it possible to set the function of the probability of destruction of nanotubes, which will make it possible to create composite materials with desired properties.

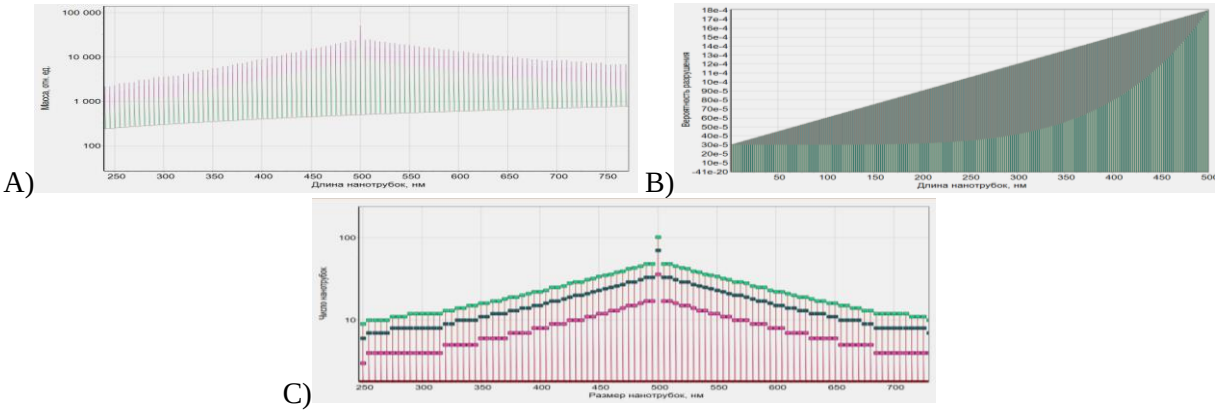

Fig.1. Graphs of the dependence of the mass on the length of nanotubes (A), the distribution of the probability of destruction (B), the size distribution of nanotubes (C).

REFERENCES

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