Disentanglement process during deformation of carbon nanotube-filled polyethylene

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Properties of polymer nanocomposites differ from properties of pure polymer. Addition of the nanoinclusions to the polymer melt affects the mobility of polymer molecules and creates additional topological limitations. The mechanical properties of the model system of a polyethylene matrix with carbon nanotubes were investigated within the method of molecular dynamics. The method of calculating the primitive path [1] was used to analyze the change in the topology of the entanglements of the polymer chains during uniaxial deformation for both systems–the pure polyethylene and the nanocomposite. It has been demonstrated that the presence of the carbon nanotubes (CNTs) made polymer matrix more disentangled. Moreover, the variation of the CNTs length affects the number and the lifetime of the entanglements. Analyzing the data, an attempt is made to find the connection between the changes in elastic properties and the pore formation [2] arising from the addition of nanoparticles dynamics and the process of disentangling interchain kinks.

[1] Sukumaran S K, Grest G S, Kremer K and Everaers R 2005 *J. Polym. Sci., Part B: Polym. Phys.* **43** 917–933
[2] Logunov M A and Orekhov N D 2018 *J. Phys.: Conf. Ser* **946** 2044