Investigation of the interaction between some polymers and carbon nanotubes

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Carbon nanotubes are ideal reinforcing materials, including for polymeric materials, because they have unique properties. Carbon nanotubes in polymer matrices have a great influence on the electrical conductivity, viscosity and other transport properties, being a hybrid of nano-scale fillers and additives [1].

A theoretical study of the interaction between the nanotubes and monomer units of several common polymers has been done. The mechanisms of these processes and their main characteristics have been identified. The possibility of joining of the monomer unit of ethylene (CH2=CH2) and propylene (CH3-CH=CH2) to the external surface of single-walled carbon (6, 6)-nanotube *have been* investigated. The research was carried out by applying the Molecular Cluster model (MC) and semi-empirical quantum-chemical MNDO scheme [2].

The process of adsorption for both cases was simulated by step-by-step approach (with a step of 0.1 Å) of monomer molecules of polyethylene or polypropylene to the carbon nanotube surface. The geometry of system was optimized on each step. The calculations have allowed to model energy curves of these processes. The research showed the most probable mechanisms of these processes and their basic characteristics. The calculated values of the adsorption energy suggested the strength of the resulting hybrid polymer material.

It was proved, that the hybrid polymer nanostructures are stable. The values of intermolecular interaction energy have been carried out. This research suggests that the reinforcement of polymer polyethylene and polypropylene matrices with carbon nanotubes is possible and efficient. This fact cans ensure the creation of new polymer nanocomposite materials with new physical and chemical properties.

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[2] Zaporotskova I.V., Carbon and noncarbon nanomaterials and composite structures on its base: the structure and electronic properties. - Volgograd: VolSU, - Volgograd, 2009.– 490.P.