Nanocomposites and nanomaterials

Influence of ferrum complex on the properties of polyurethane/carbon nanotubes composites

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Incorporation in polyurethane matrix anisometric carbonaceous fillers like carbon nanotubes could make cardinal influence (even at low amount of the filler) on resulting properties of polymer composites.

CPU was synthesized via stage of prepolymer based on 2,4-/2,6-toluenediisocyanate (80/20) and polypropylene glycol (M_w = 1000). CNTs were sonicated in dichloromethane and then added *in situ* to CPU on crosslinking stage to get CPU/CNT composites. The concentration of nanofillers was from 0,1 to 3% wt. CPU/CNT/$Fe(acac)_3$ was synthesized by adding of $Fe(acac)_3$ (1 % wt.).

It was established that for systems CPU/CNT the percolation threshold achieved at the filler content of 0.65% wt. Hereby, the level of conductivity increases by 4 orders from $4,5*10^{-11}$ S/cm to $7,8*10^{-7}$ S/cm at the CNTs contents 3%wt. This effect caused by formation of 3D percolation cluster in the bulk of polymer matrix. However, at the modification *in situ* of the systems CPU/CNTs/$Fe(acac)_3$, the percolation threshold significantly decreased to 0,02%wt. Herewith, the level of conductivity for such systems at the filler content 3%wt. is equal to $1,1*10^{-4}$ S/cm. These results were caused by catalytic effect of $Fe(acac)_3$ on the formation of the polymer matrix (the acceleration of the reaction is more than 5,5 times). Moreover, this compound forms the coordination bonds with functional PU groups. Such increasing of rate of CPU formation and coordination interaction could stabilize dispersion of nanoparticles and prevent CNT aggregation. Thermal conductivity of CPU/CNT and CPU/CNT/$Fe(acac)_3$ systems has different behavior. Increasing of concentration of CNTs in CPU/CNT leads to increment in thermal conductivity coefficient. But in case of CPU/CNT/$Fe(acac)_3$ systems the coefficient does not change and even has tendency to decrement. It can be explained by differences in structure of heat transport channels in both systems. In CPU/CNT system there is tendency to formation of secondary CNT aggregates because of rather long time of matrix formation. On the other hand in CPU/CNT/$Fe(acac)_3$ systems CNTs distributed more evenly and have thicker matrix layers between filler particles. Therefore in the latter systems phonon scattering and high thermal contact resistance between nanotubes cancels the effect of CNT addition on thermal conductivity of composites.