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The Physics of Interfacial Adhesion between a Polymer Matrix and Carbon Nanotubes (Nanofibers) in Nanocomposites

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Abstract

The aim of this study was to investigate the physics of interfacial adhesion in polymer/carbon nanotube systems. The study was carried out on polypropylene/carbon nanotube (nanofiber) nanocomposites employing fractal analysis.

Due to a high degree of anisotropy and low bending stiffness, carbon nanotubes (nanofibers) form ring-like structures in the polymer matrix of the nanocomposite, which are structural analogue of macromolecular coils of branched polymers. This allowed us to simulate the structure of polymer/carbon nanotube (nanofiber) nanocomposites as a polymer solution, using the methods of fractal physical chemistry. Using this approach we assume that macromolecular coils are represented by the ring-like structures of carbon nanotubes and the solvent is represented by the polymer matrix. The suggested model can be used to perform structural analysis of the level of interfacial interaction between the polymer matrix and the nanofiller, i.e. the level of interfacial adhesion. The analysis demonstrated that most contacts between carbon nanotubes and the polymer matrix, which determine the adhesion level, take place inside the ring-like structures. The fractal analysis showed that a decrease in the radius of the ring-like structures or their compactization increases the fractal dimension, which makes it difficult for the matrix polymer to penetrate into these structures. This results in a decrease in the number of contacts between the polymer and the nanofiller and a significant reduction of the level of interfacial adhesion. This effect can also be described as the consequence of compactization of the ring-like structures, demonstrated by the increased density. The article shows a direct correlation between the value of interfacial adhesion (dimensionless parameter b_{σ}), the number of contacts between the polymer and carbon nanotubes, and the volume of the ring-like structures, accessible for penetration by the polymer. The quantitative analysis demonstrated, that the number of interactions occurring on the surface of ring-like structures of carbon nanotubes (nanofibers) is only ~ 7–10 %. The suggested model allowed us to determine the correlation between the structure of the nanofiller in the polymer matrix and the level of interfacial adhesion for this class of nanocomposites.

The results of our study can be used to define the structure of carbon nanotubes (nanofibers) necessary to obtain the highest level of interfacial adhesion.

Keywords: nanocomposite, carbon nanotubes (nanofibers), interfacial adhesion, ring-like structures, fractal analysis.

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1. Introduction

The level of interfacial adhesion between the polymer matrix and the filler (nanofiller) is the key factor determining the properties of polymer composites (nanocomposites). The

authors [1–4] demonstrated that a high level of interfacial adhesion reinforces polymer nanocomposites, while the absence of adhesion may result in a decrease in the elastic modulus of a nanocomposite below the corresponding parameter of the matrix polymer. Today, carbon

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nanotubes (nanofibers) are considered to be among the most promising nanofillers used in polymers [5–10]. It is known [11–13], that the said nanofillers form ring-like structures in the polymer matrix which are similar to macromolecular coils due to their high degree of anisotropy and low bending stiffness. In work [13] demonstrated that the characteristics of these ring-like structures have a significant effect on both the level of interfacial adhesion and the properties of polymer nanocomposites filled with carbon nanotubes (nanofibers). Therefore, the purpose of this study was to investigate the physics of interfacial adhesion in polypropylene/carbon nanotube (nanofiber) nanocomposites.

2. Experimental

Kaplen 01030 polypropylene (PP) was used as the matrix. This type of PP is characterised by the melt flow rate of 2.3–3.6 g/10 min (the mass of polymer, in grams, flowing in 10 minutes through a standard capillary rheometer (viscometer) under specific conditions), with the weight-average molecular weight being $\sim (2-3) \times 10^5$ and the polydispersity index being 4.5.

The nanofillers were Taunite carbon nanotubes (CNTs) with 20–70 nm outer diameter, 5–10 nm inner diameter, and 2 μm length. The concentration of taunite in PP/CNT nanocomposites varied within the range of 0.25–3.0 wt%. We also used 20–30 layer carbon nanofibers (CNFs) with a diameter of 20–30 nm and a length of about 2 μm . The concentration of CNFs in PP/CNF nanocomposites varied within the range of 0.15–3.0 wt%.

PP/CNT and PP/CNF nanocomposites were prepared by mixing the components in melt on a twin screw extruder Thermo Haake, model Reomex RTW 25/42 (Germany). The mixing was performed at a temperature of 463–503 K and a screw speed of 50 rpm for 5 minutes. The testing samples were obtained by injection moulding on a Ray-Ran casting machine Test Sample Molding Apparate RR/TS MP (Taiwan) at a temperature of 503 K and a pressure of 43 MPa.

Uniaxial tension testing was performed on the samples in the shape of a two-sided spade with the size conforming to GOST 112 62-80. The tests were conducted on a universal testing machine

Gotech Testing Machine CT-TCS 2000 (Germany), at the temperature of 293 K and the strain rate of $\sim 2 \times 10^{-3} \text{ sec}^{-1}$.

3. Results and discussion

As stated above, carbon nanotubes (nanofibers) form ring-like structures in the polymer matrix of the nanocomposite, which are similar to macromolecular coils [11–15]. We can therefore describe them using established theoretical methods of both classic [6] and fractal [16] physical chemistry of polymer solutions. In the latter case, carbon nanotubes (nanofibers) are modelled as macromolecular coils, and the polymer matrix is modelled as the solvent. The fractal analysis demonstrated [16], that the number of interactions between CNTs (CNFs) and the polymer matrix n can be determined the same way as the one used for polymer solutions:

$$n \sim R_{\text{CNT}}^{D_f^{\text{PP}}}, \quad (1)$$

where R_{CNT} is the radius of the ring-like structures of CNTs (CNFs) and D_f^{PP} is the fractal dimension of the macromolecular coils of the matrix polymer (in our study, PP), which in this case represent the molecules of the solvent. R_{CNT} can be determined within the percolative model using the following equation [17]:

$$\varphi_n = \frac{\pi L_{\text{CNT}} r_{\text{CNT}}^2}{(2R_{\text{CNT}})^3}, \quad (2)$$

where φ_n is the volume fraction of the nanofiller, L_{CNT} and r_{CNT} are the length and the radius of the carbon nanotube (nanofiber) respectively.

The value of φ_n can be determined using a well-known formula [1]:

$$\varphi_n = \frac{W_n}{\rho_n}, \quad (3)$$

where W_n is the weight fraction of the nanofiller and ρ_n is its density, evaluated for the nanoparticles using [1]:

$$\rho_n = 188(D_{\text{CNT}})^{1/3}, \text{ kg/m}^3, \quad (4)$$

where D_{CNT} is the diameter of the carbon nanotube (nanofiber) in nm.

The dimension D_f^{PP} are determined for linear polymers using [19]:

$$D_f^{\text{PP}} = \frac{2d_f}{3}, \quad (5)$$

where d_f is the fractal dimension of the structure of the nanocomposite (namely, its polymer matrix) determined according to [18]:

$$d_f = (d - 1)(1 + \nu), \tag{6}$$

where d is the dimension of the Euclidean space in which the fractal is considered (apparently, in our study $d = 3$), ν is Poisson's ratio determined as a result of mechanical testing using the following [18–20]:

$$\frac{\sigma_Y}{E_n} = \frac{1 - 2\nu}{6(1 + \nu)}, \tag{7}$$

where σ_Y and E_n are the yield stress and the elastic modulus of the nanocomposite respectively.

It is known [16] that in polymer solutions the solvent penetrates into the macromolecular coil, with the process regulated by the volume of the coil accessible for penetration. Since both the macromolecular coil [16] and the ring-like structures of CNTs (CNFs) [13, 21, 22] are fractal objects, the volume of the latter structures V_{CNT} can be determined as follows [23]:

$$V_{CNT} = R_{CNT}^{D_f^{CNT}} \eta^{d - D_f^{CNT}}, \tag{8}$$

where D_f^{CNT} is the fractal dimension of the ring-like structures of CNTs (CNFs) and η is the linear scale of measurement further considered to be equal to the mean diameter of the CNTs, i.e. 45 nm.

To evaluate the dimensionality of D_f^{CNT} the following method was used [14, 15]. The calculation of R_{CNT} using equation (2) demonstrated its decrease with the growth of ϕ_n . At the maximum used values of ϕ_n , corresponding to $W_n = 3.0$ wt%, the said dependencies tend to be in the asymptotic branch, which means that the ring-like structures of CNTs or CNFs reach their minimum values R_{CNT} . Similar to the case of macromolecular coils, this means that the maximum density of the ring-like structure is reached at the maximum value of its fractal dimension D_f^{CNT} (D_f^{lim}), which is determined using the equation [24, 25]:

$$D_f^{lim} = \frac{4(d + 1)}{7}. \tag{9}$$

For $d = 3$ the value $D_f^{lim} = 2.286$.

Then, in order to estimate D_f^{CNT} an irreversible aggregation model can be used which describes the polymerization process (macromolecular

coil formation) and yields the following ratio for determining the radius of the particle aggregate R_{ag} [26–29]:

$$R_{ag} \sim c_0^{-1/(d - D_f)}, \tag{10}$$

where c_0 is the initial concentration of the aggregated particles and D_f is the fractal dimension of the aggregate.

The coefficient in ratio (10) can be determined under the following conditions: $R_{ag} = R_{CNT}$, $c_0 = \phi_n$, and $D_f = D_f^{lim}$. Values R_{CNT} and ϕ_n are applicable, when $W_n = 3.0$ wt%. The estimate obtained using this ratio demonstrated that the value D_f^{CNT} increases with the growth of ϕ_n (and a decrease in R_{CNT}) from 1.91 to 2.29 for PP/CNT nanocomposites and from 1.76 to 2.21 for PP/CNF nanocomposites.

However, due to the excluded volume effect, the polymer can not occupy the whole volume V_{CNT} , but rather occupies the available space determined by the available volume of the ring-like structures V_{CNT}^{av} , which is calculated as follows [23]:

$$V_{CNT}^{av} = V_{CNT} (3 - D_f^{CNT}). \tag{11}$$

Fig. 1 shows the ratio of the number of contacts in the studied nanocomposites between the CNTs (CNFs) and the polymer matrix n to the volume of the ring-like structures of CNTs (CNFs) V_{CNT}^{av} that can be occupied by the matrix polymer. We can see that there is a linear correlation between the said parameters which goes through the origin of the coordinates and can be described by the empirical equation

$$n = 12,1 V_{CNT}^{av}, \tag{12}$$

provided that the linear dimensions in ratios (1) and (8) are given in μm .

Thus, the number of interactions between the nanofiller and the polymer matrix n is, as expected, determined by the volume of the ring-like structures V_{CNT}^{av} , available to be occupied by the polymer which in our study is considered to be the solvent.

It is known [1] that the density of a fractal object (in our study, the density of the ring-like structures of CNTs (CNFs)) ρ_{CNT} is determined by the equation:

$$\rho_{CNT} = \rho_{dens} \left(\frac{R_{CNT}}{O} \right)^{D_f^{CNT} - d}, \tag{13}$$

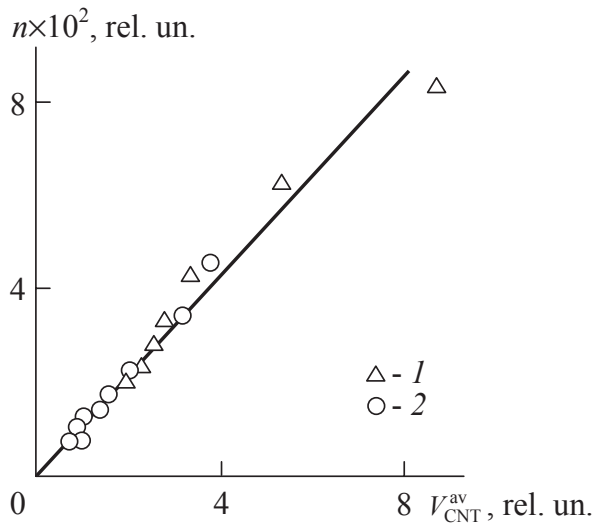


Fig. 1. The ratio of the number of contacts between the nanofiller and the polymer matrix n to the accessible volume of the ring-like structures of CNT (CNF) $V_{\text{CNT}}^{\text{av}}$ for PP/CNT (1) and PP/CNF (2) nanocomposites

where ρ_{dens} is the density of the material of the fractal object in the compact state (i.e. when $D_f^{\text{CNT}} = d$), which in our case was 2700 kg/m^3 [1], and a is the lower scaling limit of fractal behaviour assumed to be equal to D_{CNT}^* .

Fig. 2 shows the dependencies of $n(\rho_{\text{CNT}})$ for the studied nanocomposites, which demonstrate that with equal ρ_{CNT} the value of n is lower for CNFs than for CNTs. This difference is accounted for by the smaller diameter of the CNFs as compared to CNTs, which results in smaller spaces between CNFs and makes it more difficult for the macromolecular coils of PP to penetrate into the ring-like structures, since the diameter of the coils is compatible with the diameter of the CNFs.

The level of interfacial adhesion in the polymer nanocomposites can be evaluated using the dimensionless parameter b_α , which is determined according to the following ratio [1]:

$$\frac{E_n}{E_m} = 1 + 11(c\varphi_n b_\alpha)^{1.7}, \quad (14)$$

where E_n and E_m are the elastic moduli of the nanocomposite and the matrix polymer respectively (ratio E_n/E_m is usually called the reinforcement degree of the nanocomposite), c is a constant coefficient, which for the CNTs is approximately 2.86 [1].

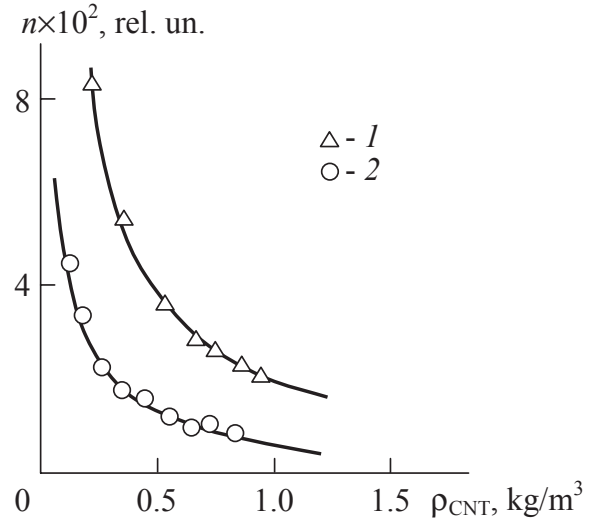


Fig. 2. Dependencies of the number of contacts between the nanofiller and the polymer matrix n on the density of the ring-like structures of CNT (CNF) ρ_{CNT} for PP/CNT (1) and PP/CNF (2) nanocomposites

Parameter b_α allows both a quantitative and qualitative gradation of the level of interfacial adhesion. Thus, when $b_\alpha = 0$, no interfacial adhesion is present; $b_\alpha = 1.0$ corresponds to perfect adhesion by Kerner; and the condition $b_\alpha > 1.0$ defines the nano-adhesion effect [1].

Fig. 3 demonstrates the dependency of the parameter b_α on the value n for PP/CNT and PP/CNF nanocomposites. As expected, the level of interfacial adhesion characterised by parameter b_α increases with a larger number of contacts between the polymer matrix and the nanofiller. The graphs in Fig. 3 have two specific features. First, the slope of the line graph $b_\alpha(n)$ is greater for CNFs as compared to CNTs. It is known [1,30] that the value b_α is the function of both the structure factor, i.e. n , and the degree of physical and/or chemical interaction between the polymer matrix and the nanofiller. The higher slope of graph $b_\alpha(n)$ for CNFs, meaning higher values of b_α for CNFs as compared to CNTs, demonstrates that physical and/or chemical interaction between PP and CNFs is stronger than the interaction between PP and CNTs. Second, graphs of $b_\alpha(n)$ are extrapolated to $b_\alpha = 0$, when n is not equal to zero. This means that for the condition $b_\alpha > 0$ (i.e. interfacial adhesion) to be implemented, we need to obtain a finite number of interactions between the polymer matrix and the nanofiller which has to be above zero.

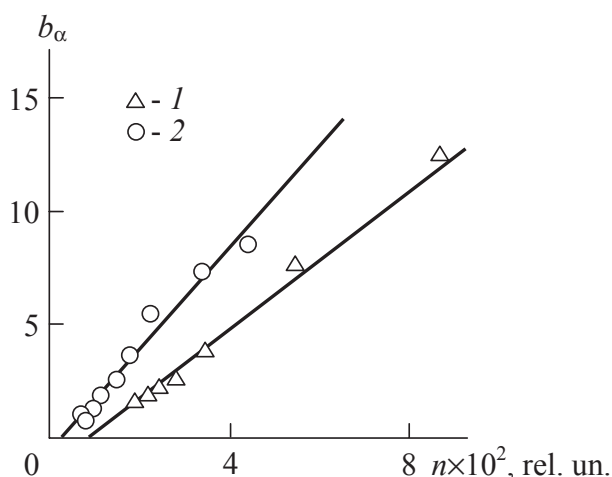


Fig. 3. Dependencies of parameter b_α on the number of contacts between the nanofiller and the polymer matrix n for PP/CNT (1) and PP/CNF (2) nanocomposites

Finally, Fig. 4 shows the dependency $b_\alpha^{1/2}(V_{\text{CNT}}^{\text{av}})$ for the studied nanocomposites (the form of the dependency was chosen so that it would allow its linearization). The figure demonstrates the growth of b_α with the increase in $V_{\text{CNT}}^{\text{av}}$, which was what we expected (Fig. 1 and 3). Once again the value of b_α with comparable $V_{\text{CNT}}^{\text{av}}$ is higher for CNFs than for CNTs, which is explained by the factors described above. The most interesting feature of the dependencies $b_\alpha^{1/2}(V_{\text{CNT}}^{\text{av}})$ is the fact that they are extrapolated to zero $b_\alpha^{1/2} \approx 0.7$ ($b_\alpha \approx 0.5$) when $V_{\text{CNT}}^{\text{av}} = 0$. Therefore, the interaction between the polymer matrix and carbon nanotubes (nanofibers) on the surface of the ring-like structures of the nanotubes (nanofibers) constitute only a comparatively small portion ($\sim 7\text{--}10\%$) of the total number. The level of interfacial adhesion is mostly determined by the interaction with the polymer penetrating into the ring-like structures of CNTs (CNFs). Therefore, the smaller radius of the said structures R_{CNT} and their corresponding compactization result in a decrease in the parameter b_α . The nano-adhesion effect ($b_\alpha > 1.0$) is observed only when the polymer penetrates into the ring-like structures of CNTs (CNFs).

It should be noted that the curvature of carbon nanotubes and their influence on the properties of nanocomposites has always been a subject of scientific studies [31–39].

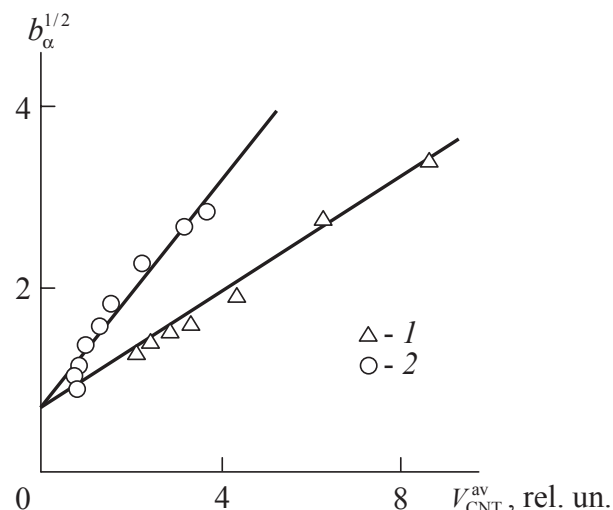


Fig. 4. Dependencies of parameter b_α on the accessible volume of the ring-like structures of CNT (CNF) $V_{\text{CNT}}^{\text{av}}$ for PP/CNT (1) and PP/CNF (2) nanocomposites

4. Conclusions

The paper suggests a structural model of creation of interfacial adhesion in polymer/carbon nanotubes (nanofibers) nanocomposites, which considers the nanofillers to be analogous to macromolecular coils and the polymer matrix to be analogous to the solvent. This model allowed us to demonstrate that most contacts between the polymer matrix and the nanofiller, determining the level of interfacial adhesion, occur within the ring-like structures of carbon nanotubes (nanofibers) when they are penetrated by the polymer. The smaller radius of the said structures makes them more compact, reduces the concentration of the polymer, and therefore reduces the level of interfacial adhesion.

Conflict of interests

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

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