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The effect of non-covalent functionalization on the interaction energy of carbon nanotubes

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Abstract

The Lennard-Jones potential function together with the continuous approximation is employed to determine the van der Waals interaction between two parallel cylindrical nanotubes. Here we determine the interaction energy between carbon nanotubes and those with non-covalent functionalization polyether ether ketone (PEEK) polymer. The distance for any two tubes does not depend on the tube radii and the number of nanotube walls. This closest distance between two surfaces for any two tubes is determined to be 0.32 nm. Furthermore, the binding energy between two tubes depends on the number of walls. Non-covalent agglomeration with polymers reduces the interaction energy between tubes and reduces agglomeration of carbon nanotubes.

1. Introduction

The improvement of polymer blends has been developed for either enhancing mechanical and electrical properties of polymers [1] or designing new composite materials [2, 3]. The dispersion of nanotubes in polyether ether ketone (PEEK) is a well-studied system [4]. PEEK is a thermoplastic with excellent mechanical and chemically resistant properties [5], that is used in spinal fusion devices, and has many applications in the aerospace and automotive industries [5, 6]. Henneuse-Boxus *et al* [7] consider the surface topologically functionalization of PEEK films, and determine the percentage of atomic compositions for twenty samples of PEEK. Here, we employ the atomic compositions data given in [7] to determine the Lennard-Jones parameters for the van der Waals calculation.

Carbon nanotubes have attracted much attention as a means to create novel nano-devices. This is due to their small size and their unique properties including mechanical, electronic, high flexibility and low friction [8–10]. One of the most important issues in producing nanocomposites and devices is to understand the interatomic van der Waals potential energy behaviour between two carbon nanostructures. Girifalco and collaborators [11, 12] employ the Lennard-Jones potential function to determine universal graphitic systems. Zheng *et al* [9, 10] also use the Lennard-Jones function to determine the energy for multi-walled carbon nanotubes and propose a gigahertz frequency oscillator. The present authors determine analytically the energy for such nano-scaled carbon based systems [13].

In terms of the combination of carbon nanotubes and PEEK, Nayak *et al* [14] study the dispersion of carbon nanotubes with silicon carbide coating on carbon nanotubes in PEEK, and find that coated carbon nanotubes improve the mechanical properties of PEEK and reduce the agglomeration of polymer chains. Tishkova *et al* [15] investigate the dispersion of single-walled, double-walled and multi-walled carbon nanotubes in PEEK, and conclude that the dispersion depends on the number of walls, and single-walled carbon nanotubes show a different dispersion behaviour than multi-walled carbon nanotubes. Moreover, the coating of ultra-high molecular weight polyethylene (UHMWPE) on carbon nanotubes improves the friction and wear of PEEK [16].

In this paper, the van der Waals interaction between carbon nanotubes and on non-covalent functionalization of PEEK is investigated. The Lennard-Jones potential function and the continuous assumption are employed to determine the total interaction energy of the system. In contrast to using a computational technique to find the energy behaviour, our aim here is to obtain an analytical expression as a function of the nanotube radius and the atomic composition of the polymer. Consequently, the van der Waals energy between a pair of nanotubes can be computed for a wide variety of differing situations.

In particular, we investigate the interaction energy between a parallel pair of coated and uncoated nanotubes to demonstrate an alignment of carbon nanotubes in the polymer matrix. This is an example of a theoretical observation that might be used to determine the energy behaviour of other polymer-based composites such as a composite system involving epoxy and carbon nanotubes [17]. Most agglomerations between two tubes are more complex but here we focus on understanding the effect of functionalization on agglomeration. An ideal case is assumed which can be modeled in an analytic form.

Both the Lennard-Jones potential function and the continuous approximation are detailed in the following section. Mathematical derivations for the interaction energies between an atom and an infinite tube, between two parallel tubes, and between two concentric tubes are presented in section 2. Results and discussion are given in section 3, and finally, conclusions are presented in section 4.

2. Interaction energy

We employ the Lennard-Jones potential and the continuous approximation to determine the molecular interatomic energy between two molecules. We assume the 6–12 Lennard-Jones potential is given by

$$\Phi = -\frac{A}{\rho^6} + \frac{B}{\rho^{12}},$$

where ρ denotes the distance between two atoms. According to the study of Rappé *et al* [18] (see equation (20) [18]), $A = 2\epsilon\sigma^6$ and $B = \epsilon\sigma^{12}$ are respectively the attractive and repulsive constants, and where ϵ is the energy well depth and σ is the inter-atomic distance. The potential is minimum at the distance $\sigma = (2B/A)^{1/6}$.

The continuous approach assumes that atoms at discrete locations on a molecule are averaged over the surface of the molecule, which means that summations over all atoms can be replaced by surface integrals. The molecular interatomic energy is then obtained by evaluating integrals over the surface of each molecule, given by

$$E = \eta_1 \eta_2 \int_{S_1} \int_{S_2} \left(-\frac{A}{\rho^6} + \frac{B}{\rho^{12}} \right) dS_2 dS_1,$$

where η_1 and η_2 represent the mean or average atomic density of atoms over the surface of each molecule. Further, by writing

$$I_n = \int_{S_1} \int_{S_2} \rho^{-2n} dS_2 dS_1, \quad (n = 3, 6), \quad (1)$$

the above equation can then be written as

$$E = \eta_1 \eta_2 (-AI_3 + BI_6). \quad (2)$$

In this study, we first consider the interaction energy between an atom at the point P and an infinite cylindrical surface. The atom at point P is then assumed to be located on another cylindrical tube, and then the second cylindrical surface integral is evaluated to determine the total interaction energy between two nanotubes.

2.1. Interaction energy between infinite tube and point

Here we assume that the tube of radius a_1 is of infinite length, centred at the origin as shown in figure 1, and there is an atom located at a distance δ_1 in the x -direction. The distance between the atom at the point P and an arbitrary point on the tube is given by

$$\begin{aligned} \rho^2 &= (a_1 \cos \theta_1 - \delta_1)^2 + (a_1 \sin \theta_1)^2 + z_1^2 \\ &= (\delta_1 - a_1)^2 + 4a_1 \delta_1 \sin^2(\theta_1/2) + z_1^2, \end{aligned}$$

where we have used $\cos 2\theta = 1 - 2\sin^2 \theta$ and we assume that $\delta_1 > a_1$.

The integral I_n defined by (1) now becomes

$$I_n = a_1 \int_{-\infty}^{\infty} \int_{-\pi}^{\pi} \frac{1}{[(\delta_1 - a_1)^2 + 4a_1 \delta_1 \sin^2(\theta_1/2) + z_1^2]^n} d\theta_1 dz_1,$$

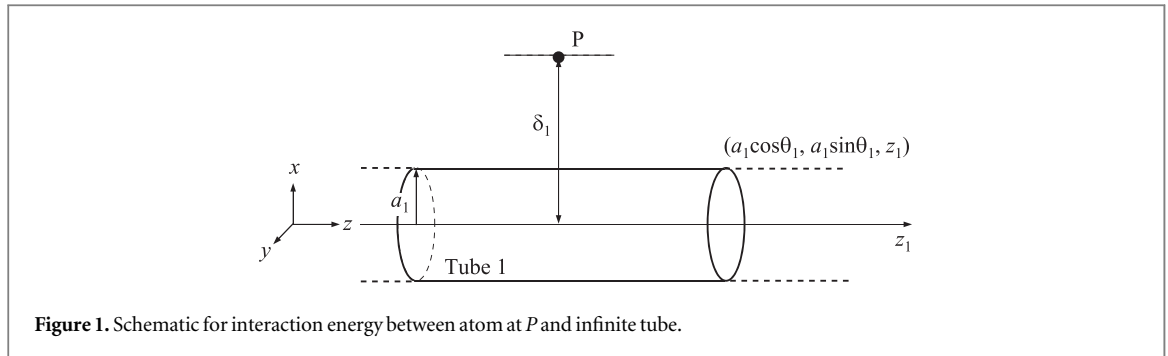


Figure 1. Schematic for interaction energy between atom at P and infinite tube.

and on letting $\lambda^2 = (\delta_1 - a_1)^2 + 4a_1\delta_1 \sin^2(\theta_1/2)$ and substituting $z_1 = \lambda \tan \psi$, we may deduce

$$\begin{aligned} I_n &= a_1 \int_{-\pi/2}^{\pi/2} \int_{-\pi}^{\pi} \frac{\lambda \sec^2 \psi}{(\lambda^2 + \lambda^2 \tan^2 \psi)^n} d\theta_1 d\psi \\ &= a_1 \int_{-\pi/2}^{\pi/2} \cos^{2n-2} \psi d\psi \int_{-\pi}^{\pi} \lambda^{1-2n} d\theta_1. \end{aligned}$$

Next we use the integral form of the beta function

$$\int_0^{\pi/2} \sin^p \theta \cos^q \theta d\theta = \frac{1}{2} B\left(\frac{p+1}{2}, \frac{q+1}{2}\right),$$

and substitute $t = \sin^2(\theta_1/2)$, so that the integral I_n can be written as

$$I_n = \frac{2a_1}{(\delta_1 - a_1)^{2n-1}} B\left(n - \frac{1}{2}, \frac{1}{2}\right) \int_0^1 t^{-1/2} (1-t)^{-1/2} (1-\mu t)^{1/2-n} dt, \quad (3)$$

where $\mu = -4\delta_1 a_1 / (\delta_1 - a_1)^2$.

Euler's integral formula for the hypergeometric function is given by

$$F(a, b; c; z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 t^{b-1} (1-t)^{c-b-1} (1-zt)^{-a} dt, \quad (4)$$

and, when $c = 2b$ a quadratic transformation can be used to give

$$F(a, b; 2b; z) = \left[\frac{1 + (1-z)^{1/2}}{2} \right]^{-2a} F\left(a, a-b + \frac{1}{2}; b + \frac{1}{2}; \left[\frac{1 - (1-z)^{1/2}}{1 + (1-z)^{1/2}} \right]^2\right). \quad (5)$$

On employing Euler's integral formula and the above quadratic transformation for the hypergeometric, respectively, equation (3) becomes

$$\begin{aligned} I_n &= \frac{2\pi a_1}{(\delta_1 - a_1)^{2n-1}} B\left(n - \frac{1}{2}, \frac{1}{2}\right) F\left(n - \frac{1}{2}, \frac{1}{2}; 1; -\frac{4\delta_1 a_1}{(\delta_1 - a_1)^2}\right) \\ &= \frac{2\pi a_1}{\delta_1^{2n-1}} B\left(n - \frac{1}{2}, \frac{1}{2}\right) F\left(n - \frac{1}{2}, n - \frac{1}{2}; 1; \frac{a_1^2}{\delta_1^2}\right). \end{aligned} \quad (6)$$

Therefore, the interaction energy between an atom at the point P and an infinite cylindrical nanotube becomes simply

$$\begin{aligned} E_{cp} &= \eta_1 \left[-\frac{2\pi a_1 A}{\delta_1^5} B\left(\frac{5}{2}, \frac{1}{2}\right) F\left(\frac{5}{2}, \frac{5}{2}; 1; \frac{a_1^2}{\delta_1^2}\right) + \frac{2\pi a_1 B}{\delta_1^{11}} B\left(\frac{11}{2}, \frac{1}{2}\right) F\left(\frac{11}{2}, \frac{11}{2}; 1; \frac{a_1^2}{\delta_1^2}\right) \right] \\ &= \pi^2 \eta_1 a_1 \left[-\frac{3A}{4\delta_1^5} F\left(\frac{5}{2}, \frac{5}{2}; 1; \frac{a_1^2}{\delta_1^2}\right) + \frac{63B}{128\delta_1^{11}} F\left(\frac{11}{2}, \frac{11}{2}; 1; \frac{a_1^2}{\delta_1^2}\right) \right], \end{aligned} \quad (7)$$

where η_1 is the mean atomic density of the tube.

2.2. Interaction energy between two parallel cylinders

In this section, we consider the interaction energy between two parallel nanotubes where the atom at the point P , from the previous section, is assumed to be an arbitrary point on the second nanotube as shown in figure 2. Since there are infinitely many atoms on the two infinite tubes, the total energy of the system will necessarily tend to infinity, and therefore only the interaction energy per unit length will be determined. However, the θ integral must still be evaluated for the second tube. Consequently, the interaction energy per unit length is

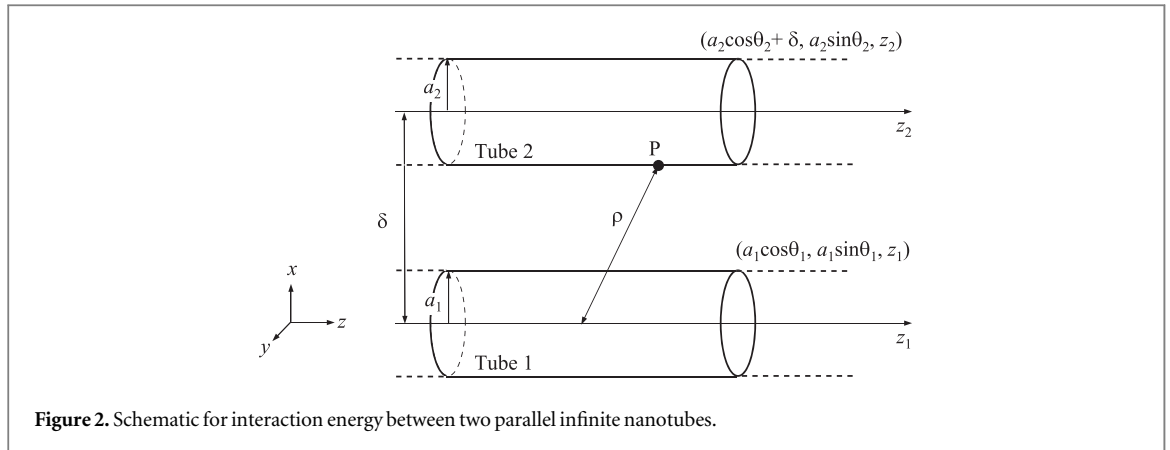


Figure 2. Schematic for interaction energy between two parallel infinite nanotubes.

$$E_{cc} = \eta_2 a_2 \int_{-\pi}^{\pi} (-AI_3 + BI_6) d\theta_2$$

$$= 2\pi\eta_1\eta_2 a_1 a_2 (-AJ_3 + BJ_6), \quad (8)$$

where I_n for $n = 3$ and 6 are defined by (6), η_2 is the mean atomic density of the second tube, and J_n for $n = 3$ and 6 are defined by

$$J_n = B\left(n - \frac{1}{2}, \frac{1}{2}\right) \int_{-\pi}^{\pi} \rho^{1-2n} F\left(n - \frac{1}{2}, n - \frac{1}{2}; 1; \frac{a_1^2}{\rho^2}\right) d\theta_2. \quad (9)$$

The distance from the centre of the first tube to a typical point on the second tube, previously δ_1 , is given by

$$\rho^2 = (a_2 \cos \theta_2 + \delta)^2 + (a_2 \sin \theta_2)^2 = (\delta - a_2)^2 + 4a_2 \delta \sin^2(\theta_2/2),$$

where a_2 is the radius of the second tube and δ is the distance between their centres.

We use the series form of the hypergeometric function which is given by

$$F\left(n - \frac{1}{2}, n - \frac{1}{2}; 1; \frac{a_1^2}{\rho^2}\right) = \sum_{k=0}^{\infty} \frac{(n - 1/2)_k (n - 1/2)_k}{(1)_k k!} \frac{a_1^{2k}}{\rho^{2k}},$$

to obtain

$$J_n = B\left(n - \frac{1}{2}, \frac{1}{2}\right) \sum_{k=0}^{\infty} \frac{(n - 1/2)_k (n - 1/2)_k}{(1)_k k!} a_1^{2k} \int_{-\pi}^{\pi} \rho^{1-2n-2k} d\theta_2.$$

For convenience, we now define

$$K_p = \int_{-\pi}^{\pi} \rho^{1-2p} d\theta_2$$

$$= \int_{-\pi}^{\pi} [(\delta - a_2)^2 + 4a_2 \delta \sin^2(\theta_2/2)]^{1/2-p} d\theta_2$$

$$= 2(\delta - a_2)^{1-2p} \int_0^1 t^{-1/2} (1-t)^{-1/2} \left[1 + \frac{4a_2 \delta}{(\delta - a_2)^2} t\right]^{1/2-p} dt,$$

where $t = \sin^2(\theta_2/2)$, and again we use Euler's integral formula for the hypergeometric function given by (4) and the quadratic transformation defined by (5), and we may deduce

$$K_p = 2\pi(\delta - a_2)^{1-2p} F\left(p - \frac{1}{2}, \frac{1}{2}; 1; -\frac{4a_2 \delta}{(\delta - a_2)^2}\right)$$

$$= 2\pi\delta^{1-2p} F\left(p - \frac{1}{2}, p - \frac{1}{2}; 1; \frac{a_2^2}{\delta^2}\right).$$

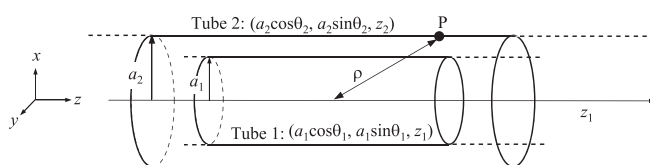


Figure 3. Schematic for interaction energy between two concentric nanotubes.

Hence, the integral J_n can be written as

$$\begin{aligned} J_n &= 2\pi B\left(n - \frac{1}{2}, \frac{1}{2}\right) \sum_{k=0}^{\infty} \frac{(n - 1/2)_k (n - 1/2)_k}{(k!)^2} a_1^{2k} \delta^{1-2n-2k} F\left(n + k - \frac{1}{2}, n + k - \frac{1}{2}; 1; \frac{a_2^2}{\delta^2}\right) \\ &= \frac{2\pi}{\delta^{2n-1}} B\left(n - \frac{1}{2}, \frac{1}{2}\right) \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \left[\frac{(n - 1/2)_k (n + k - 1/2)_l}{k! l!} \right]^2 \left(\frac{a_1}{\delta}\right)^{2k} \left(\frac{a_2}{\delta}\right)^{2l} \\ &= \frac{2\pi}{\delta^{2n-1}} B\left(n - \frac{1}{2}, \frac{1}{2}\right) \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \left[\frac{(n - 1/2)_{k+l}}{k! l!} \right]^2 \left(\frac{a_1}{\delta}\right)^{2k} \left(\frac{a_2}{\delta}\right)^{2l}. \end{aligned}$$

From the series form of Appell's hypergeometric function of the fourth kind F_4 (see for example [19]), we may write

$$J_n = \frac{2\pi}{\delta^{2n-1}} B\left(n - \frac{1}{2}, \frac{1}{2}\right) F_4\left(n - \frac{1}{2}, n - \frac{1}{2}, 1, 1; \frac{a_1^2}{\delta^2}; \frac{a_2^2}{\delta^2}\right). \quad (10)$$

Finally, the interaction energy between two parallel cylinders can be obtained by substituting (10) into (8) to yield

$$E_{cc} = \pi^3 a_1 a_2 \eta_1 \eta_2 \left[-\frac{3A}{2\delta^5} F_4\left(\frac{5}{2}, \frac{5}{2}, 1, 1; \frac{a_1^2}{\delta^2}; \frac{a_2^2}{\delta^2}\right) + \frac{63B}{64\delta^{11}} F_4\left(\frac{11}{2}, \frac{11}{2}, 1, 1; \frac{a_1^2}{\delta^2}; \frac{a_2^2}{\delta^2}\right) \right]. \quad (11)$$

2.3. Interaction energy between two concentric cylinders

For the special case when $\delta = 0$ as shown in figure 3, we obtain the case of concentric nanotubes where $\rho^2 = a_2^2$, and (9) becomes

$$\begin{aligned} J_n &= B\left(n - \frac{1}{2}, \frac{1}{2}\right) \int_{-\pi}^{\pi} a_2^{1-2n} F\left(n - \frac{1}{2}, n - \frac{1}{2}; 1; \frac{a_1^2}{a_2^2}\right) d\theta_2 \\ &= 2\pi B\left(n - \frac{1}{2}, \frac{1}{2}\right) a_2^{1-2n} F\left(n - \frac{1}{2}, n - \frac{1}{2}; 1; \frac{a_1^2}{a_2^2}\right), \end{aligned}$$

and the interaction energy between two concentric cylinders is given by

$$E_{co} = \pi^3 \eta_1 \eta_2 a_1 a_2 \left[-\frac{3A}{2a_2^5} F\left(\frac{5}{2}, \frac{5}{2}; 1; \frac{a_1^2}{a_2^2}\right) + \frac{63B}{64a_2^{11}} F\left(\frac{11}{2}, \frac{11}{2}; 1; \frac{a_1^2}{a_2^2}\right) \right]. \quad (12)$$

We comment that equations (11) and (12) can be readily evaluated using standard algebraic packages such as MAPLE.

3. Results and discussion

The interaction energies between any two parallel carbon nanotubes and non-covalently functionalized nanotubes are now examined. We assume that the total interaction energy of the system arises only from the atomic components on the nanotube surface, such as polymer coating, and that there is no energy contribution arising from the underlying tube base material. This is because polymer coated carbon nanotubes are stable in the mixture, and the polymer on the tube surface already accommodates the energy contribution from the underlying tube base. Furthermore, it is justified by the short range interaction of the Lennard-Jones potential with the cutoff distance of around 9 Å [20]. Consequently, if we ignore the underlying carbon base, we may consider the interaction energy between carbon nanotubes and PEEK tubes.

Here, the total interaction energy per unit length is determined. The Lennard-Jones parameters are taken from the work of Rappé *et al* [18]. For any system involving two atomic elements, we follow normal practice and utilize the empirical mixing rules for ϵ and σ , which are $\epsilon_{1,2} = \sqrt{\epsilon_1 \epsilon_2}$ and $\sigma_{1,2} = (\sigma_1 + \sigma_2)/2$, where 1 and 2

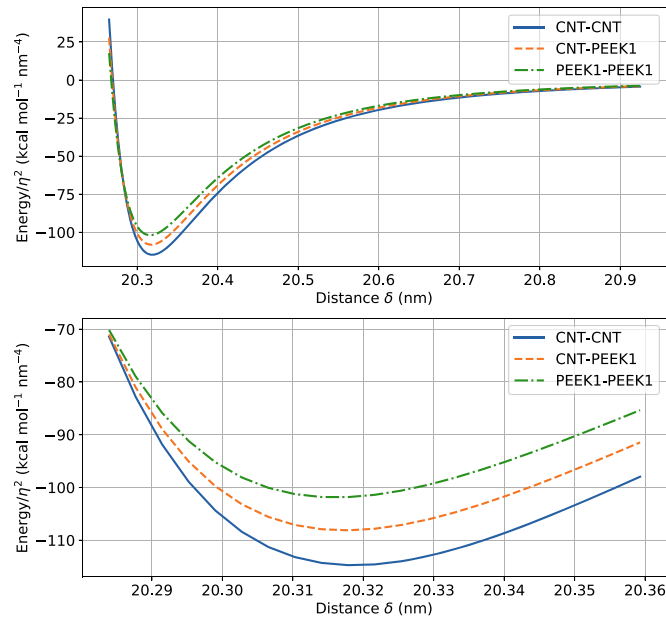


Figure 4. Interaction energy per mean atomic density squared for three cases of interactions.

refer to atomic types 1 and 2, respectively [21]. The mean atomic densities of the tubes are assumed to be equal and only the proportion of atomic types that affect the Lennard-Jones constants, $A_{1,2} = 2\sqrt{\epsilon_1\epsilon_2}[(\sigma_1 + \sigma_2)/2]^6$ and $B_{1,2} = \sqrt{\epsilon_1\epsilon_2}[(\sigma_1 + \sigma_2)/2]^{12}$ are considered.

Henneuse-Boxus *et al* [7] report the atomic compositions of twenty entries for functionalization of PEEK. In this study we consider three examples which are entries 1, 7 and 15, and the percentages for each atom can be found in table 1 of [7].

For example, the Lennard-Jones constants between the carbon nanotube and the tube coated with PEEK entry 1 are given by

$$A_{C,P1} = \left(\frac{83.31}{100}\right)A_{C,C} + \left(\frac{16.69}{100}\right)A_{C,O} + \left(\frac{0}{100}\right)A_{C,N} + \left(\frac{0}{100}\right)A_{C,F} + \left(\frac{0}{100}\right)A_{C,S},$$

$$B_{C,P1} = \left(\frac{83.31}{100}\right)B_{C,C} + \left(\frac{16.69}{100}\right)B_{C,O} + \left(\frac{0}{100}\right)B_{C,N} + \left(\frac{0}{100}\right)B_{C,F} + \left(\frac{0}{100}\right)B_{C,S},$$

where the contribution of carbon atoms on the carbon nanotube sums to 1, and the coefficients of each term are the atomic compositions of PEEK entry 1 (see table 1 in [7]).

Figure 4 shows the interaction energy between two nanotubes of single-walled carbon nanotubes (SWNTs), or tubes with PEEK on its surface, or one SWNT with one PEEK tube where their radii are assumed to be 10 nm. PEEK tube means that the lower lying SWNT is not taken into account. We find that the strongest binding energy occurs for the case of two carbon nanotubes due to the larger value of the energy well depth ϵ for carbon atoms. On the other hand, the lowest binding energy occurs for the interaction energy of two PEEK tubes. Therefore, mixing carbon nanotubes into a polymer matrix may reduce the agglomeration of SWNTs. We comment that the energy behaviour arising from the other entries of PEEK given in [7] is similar, and only the energy profiles for PEEK entry 1 are shown in figure 4.

In terms of the equilibrium distance δ_0 , which is the distance between the centres of two nanotubes at the minimum energy, we determine δ_0 for each pair of nanotubes and their numerical values are given in table 1. The closest inter-spacing between two nanotube surfaces may be obtained as $\delta_0 - 20$ nm where we obtain the value of 0.32 nm for all cases studied here.

We also investigate how the change of radii of nanotubes affect their interaction energy and the equilibrium inter-spacing distance. To do this, we use the pair of carbon nanotube and nanotube functionalized with PEEK entry 1. We assume that the two tubes have equal radius and this radius is then varied from 5, 10, 15 and 20 nm. The inter-spacing distance between the two tubes can be obtained from $\delta - 2a$, where a is the tube radius.

The graph between interaction energy and inter-spacing distance is shown in figure 5. The binding energy is stronger as the radius increases. In addition, the inter-spacing distance at which the binding energy between the two tubes is strongest is largely independent of the tube radius, and this distance is around 0.32 nm. We comment that the same result is also obtained for smaller carbon nanotubes of radii 1 – 10 nm.

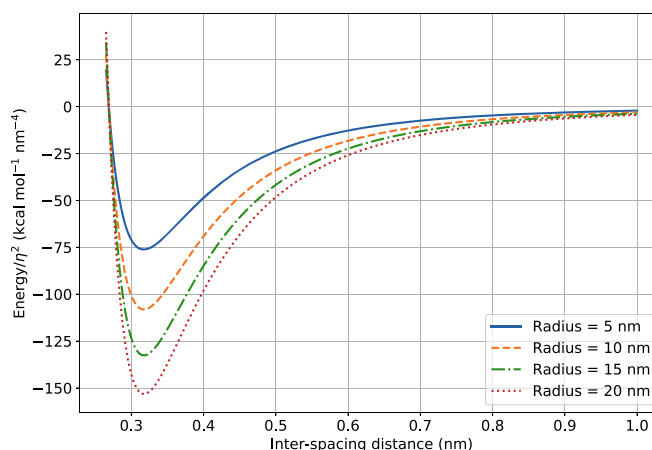


Figure 5. Interaction energy per mean atomic density squared for PEEK entry 1 tube and carbon nanotube with different radii.

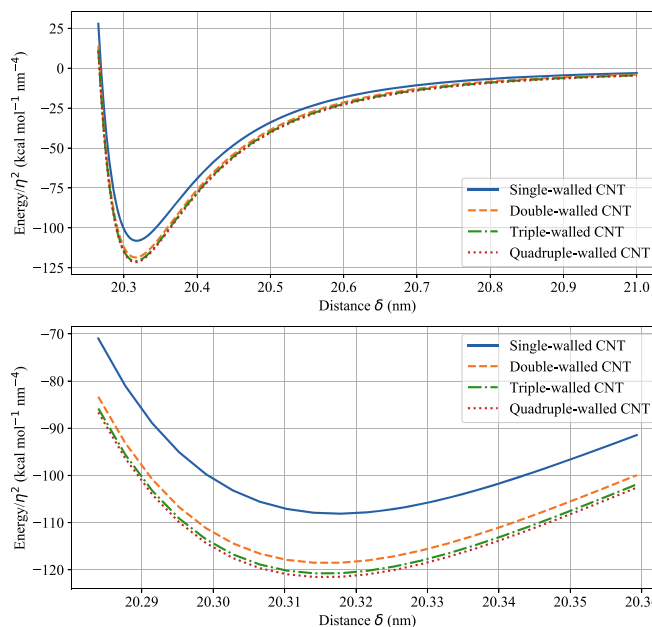


Figure 6. Interaction energy per mean atomic density squared for PEEK entry 1 tube and carbon nanotubes with different wall numbers.

Table 1. Equilibrium distance δ_0 (nm) for each pair of nanotubes of radii 10 nm.

	Carbon	PEEK entry 1	PEEK entry 7	PEEK entry 15
Carbon	20.318 7	20.317 3	20.316 9	20.317 2
PEEK entry 1	—	20.316 0	20.315 3	20.315 8
PEEK entry 7	—	—	20.315 2	20.315 7
PEEK entry 15	—	—	—	20.315 7

We further investigate the effect of the number of walls of carbon nanotube on the interaction energy. Here, the tube functionalized with PEEK and the outer most layer of the carbon nanotube are assumed to have radii of 10 nm. On using the energy expression for the interaction between two concentric nanotubes detailed in section 2.3, the equilibrium spacing between two adjacent carbon nanotube walls is obtained as 0.385 nm. Consequently, the radii of the inner layers of the carbon nanotubes decrease by 0.385 nm for each layer. Figure 6 shows the energy between PEEK entry 1 tube interacting with carbon nanotubes with different numbers of walls.

We first note that the equilibrium inter-spacing distances for the four cases appear to be equal at around 0.32 nm. This suggests that the equilibrium inter-spacing distance is independent of the number of carbon nanotube walls.

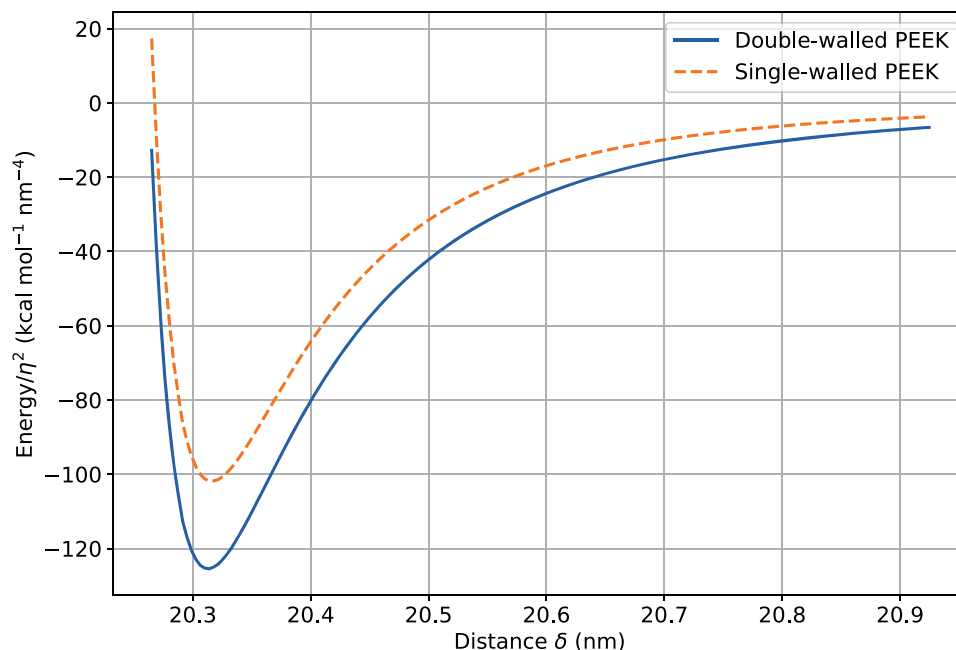


Figure 7. Interaction energy per mean atomic density squared for single-walled PEEK entry 1 tubes and double-walled tubes coated with PEEK entry 1.

As for of the binding energy, it evidently increases as the number of walls increases. However, increasing the number of walls to three or more does not significantly improve the binding energy. This agrees with the fact that the van der Waals energy is a short-range interaction and the cutoff distance is 9 Å [20], which is approximately two layers of the carbon nanotube plus the inter-spacing distance between the two tubes. Therefore, in terms of the energy calculation, we predict that the double-walled and multi-walled carbon nanotubes have the same agglomeration behaviour which is consistent with reference [15].

Next, we compare the energies between two single-walled PEEK entry 1 tubes and two double-walled tubes coated with PEEK entry 1 as shown in figure 7. In the first case, both single-walled PEEK entry 1 tubes are assumed to have radii of 10 nm. The graph between the energy and the distance δ between the centers of the tubes is shown as the (red) dotted curve in figure 7. In the second case, we have two carbon nanotubes coated with PEEK entry 1 whose radii of the outermost layers are 10 nm. The inner wall of each tube is assumed to be a cylindrical carbon tube with a radius $10 - 0.385 = 9.615$ nm. The graph in this case is shown as the (blue) solid curve in the same figure. Again, we observe a larger binding energy for the case of the double-walled tubes.

4. Summary

An analytical expression is derived to determine the interaction energy between a pair of parallel coated and uncoated cylindrical nanotubes. The Lennard-Jones potential function is employed to determine the atomic interaction energy and the continuous approximation is utilized to calculate the total energy of the system. The analytical expression so obtained can be written in terms of the beta function and the hypergeometric function.

On assuming that the nanotube radii are 10 nm, we determine the van der Waals interaction energy between two nanotubes. We find that bare carbon nanotubes give the strongest binding energy as compared to functionalized CNTs. The equilibrium distance between the closest surfaces of the two nanotubes is obtained as 0.32 nm. Our results suggest that this value does not depend on the tube radius nor on the number of carbon nanotube walls.

Double- and multi-walled CNTs have a larger interaction energy than single-walled CNTs which makes them harder to disperse in a polymer matrix. Clearly non-covalent functionalization reduces the tube interaction energy and favours dispersion of the CNTs in the polymer matrix.

The main outcome of this work is that the CNT interaction is reduced with PEEK on its surface and that this interaction depends on the first two walls of the CNTs. Further it is shown that the radius dependence can be neglected and the equilibrium distance is similar to that found between two layers in graphite. We note that under experimental conditions the CNT tubes may not have complete PEEK layers.

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