

Influences of the Nanoparticles Related Parameters on the Tensile Strength of Polymer Nanocomposites

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ABSTRACT

In this study, a comprehensive model has been proposed in order to predict the tensile strength of nanocomposites considering the effects of the random orientation of nanoparticles, the properties of the polymer/particle interphase region and also the inevitable aggregation/agglomeration phenomenon. The model was structured based on the nanoparticle shape (e. g. platelet, cylindrical and spherical) so it could perfectly demonstrate the random orientation. It was revealed that neglecting the aggregation/agglomeration of the nanoparticles ($\chi = 0$) increased the prediction error to about 12 % while the $\chi = 0.07$ % decreased the error to about 7-9 % for samples with low contents of nanoparticles (< 0.5 Vol.). The model was also applicable to the case of nanocomposites containing high contents of nanoparticles (> 1 % Vol.) which demonstrated its advantage, compared to other similar models, to predict the tensile strength in a wide range of nanoparticle contents (prediction error < 10 %). Moreover, the model was completely capable of characterizing the polymer/particle interphase regardless of the polymer type and the shape of the nanoparticles. The model verification was accomplished by comparing its predictions with the tensile test results for the prepared nanocomposite samples of different compositions (Polystyrene/Silica, Polystyrene/Graphene Oxide and Polystyrene/Carbon nano-tubes) and data from the literature. Also, the samples were subjected to TEM in order to qualitatively evaluate the behavior of the Nanoparticles with different shapes in the polystyrene matrix.

1. Introduction

The application of nanoparticles in the polymer matrices has been always an interesting topic for researchers as a practical method for enhancing the mechanical properties of polymers [1-9]. The superiority of the nanoparticles in comparison with the

micro/macro particles arises from their high specific surface area which lets them have a significant impact on the performance of the nanocomposite against the exerted stress [10-16]. However, the bonding of the polymer chains to the surface of the nanoparticles, due to the presence of different functional groups,

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is known to be responsible for the changes of many characteristics of the base polymer matrix [17-19]. The bonding causes the formation of polymer/particle interphase region of which the thickness does not exceed the radius of gyration of the polymer chains [20-23]. Therefore, compared to that of the size of the nanoparticle, the effect of the region on the mechanical properties of the system is definitely not negligible.

There are many studies that have evaluated the effect of the polymer/particle interphase on the mechanical properties of the nanocomposites however, the actual characteristics of the interphase are still unknown [19, 24-29]. The nanoparticle shape is also an effective parameter in defining the mechanical properties of the polymer nanocomposites [9, 24, 30]. For instance, the random orientation of the platelet and cylindrical nanoparticles should be definitely considered while it can be neglected in the case of spherical nanoparticles. On the other hand, the structure of the polymer/particle interphase around the nanoparticles is completely dependent on its shape and the superficial functional groups. The other affecting parameter on the mechanical properties of the nanoparticles is the aggregation/agglomeration phenomenon of the nanoparticles which has been always tried to be avoided because it turns the clusters of the so-called reinforcing particles into weak spots [12, 21, 31]. Considering the inevitability of the aggregation/agglomeration of the nanoparticles at any amount, it has been always tried to characterize the formed clusters via interpreting the properties of the actual systems using specific models [21, 32, 33].

As mentioned before, nanoparticles are very effective in enhancing the

physical/mechanical properties of the polymer bases and therefore, many studies have been performed in order to investigate these systems using both experimental/analytical methods [19, 34-38]. The mechanical properties of this group of materials (e. g. tensile modulus, tensile strength, etc.) are some of the main and important subjects in the modeling field for predicting the mechanical properties of the system [19, 24, 33, 38-40].

As a result, in this study it has been tried to design a comprehensive model that could predict the tensile strength of polymer nanocomposites considering some very effective parameters such as the shape of nanoparticles, the random orientation, the effects of the polymer/particle interphase and aggregation/agglomeration. Consequently, the presented model was capable of predicting the tensile strength of polymer nanocomposites in a wide range of nanoparticles content which is indeed a significant advantage in comparison with other similar models (Prediction error < 10 %). On the other hand, as a very important achievement, it was also possible to define the characteristics of polymer/particle interphase region by coupling the model equations with the actual tensile test results which helped to better understand the response mechanism of the nanocomposites against the exerted stress. The model prediction results were verified by comparing them with the tensile test results of some prepared nanocomposite samples, (Polystyrene/Silica, Polystyrene/Graphene Oxide and Polystyrene/Carbon nano-tubes) and some other data from the literature. Furthermore, the behavior of the nanoparticles in the polymer matrix was qualitatively evaluated using TEM in order to ensure the random orientation of platelet and

cylindrical nanoparticles.

2. Experimental

2.1. Materials

Polystyrene (PS) (density = 1.047 g/mL, CAS No.: 182427) and carbon nanotubes (CNT) (D×L: 2-10 nm × 0.5-2 μm, CAS No. 652482) were purchased from Sigma Aldrich. Graphene oxide (GO) (thickness: 1-10 nm, size: 2-10 μm) was purchased from Nanowerk Co. and Aerosil fumed silica (SI) (OX-50) was kindly provided by Degussa.

2.2. Sample preparation

CNT nanoparticles were first ball-milled for 1 h in order to reduce their length and then used as nanofillers. All PS/CNT, PS/GO, PS/SI nanocomposites samples were prepared in an internal mixer (Brabender Plasticorder W50EHT) at suitable temperatures and then formed into suitable pieces, via compression molding at 10 Mpa, for the tensile tests. The amounts of the different nanoparticles in the samples were 1, 2, 3 or 4 vol. %.

2.3. Characterization methods

The prepared samples were subjected to the tensile test (Zwick/Roell tensile testing machine) according to ISO 527. The results were reported based on testing at least 4 samples of each composition. The behavior of the different nanoparticles in the prepared samples was qualitatively investigated using the TEM device (Leo 906, Zeiss, Germany).

3. Modeling method

As mentioned before, there are some effective parameters which are essential to be considered in the modeling of the nanocomposites (e. g. random orientation, aggregation/agglomeration, polymer/particle interphase effect, etc.). Though, the random orientation of nanoparticles can be neglected

in the case of particulate polymer nanocomposites containing spherical nanoparticles which significantly simplifies the modeling procedure [21]. As it is illustrated in Figure 1, the platelet and cylindrical nanoparticles tend to be oriented towards different directions which drastically affect the tensile strength in the direction of the applied force of the exerted force. Besides, the shape of the nanoparticles should be also considered for categorizing the modeling procedure and better addressing the details.

3.1. Nanocomposites containing platelet nanoparticles

The schematic of the model structure is presented in Figure 2. As it is clear, the model consists of nanoparticle, interphase regions and also a unity cube which represents the polymer matrix. Also, the angle θ defines the random orientation of the nanoparticles toward the direction of the exerted stress.

All model parameters are to be defined based on the actual quantitative values of the systems as follows:

$$\begin{cases} \varphi'_d = k^2 z \\ k_1 k_2 = \varphi'_d (1 - \chi) 2t A_T \\ 1 - (k_1 k_2)^2 = \varphi'_m \end{cases} \quad (1)$$

where, φ'_d and φ'_m are the actual volume fractions of the nanoparticles and the polymer phase respectively, χ denotes the aggregation percentage, A_T is the total surface area of the nanoparticles and t is the thickness of the interphase region.

According to the Zare's model, it is possible to calculate the tensile strength of the polymer nanocomposites at $\theta = 0^\circ$ as follows [21]:

$$\sigma_{cT} A_c = \sigma_{mT} A_{mT} + \sigma_{iT} A \quad (2)$$

where, σ_{cT} , σ_{mT} , and σ_{iT} are the tensile strength of nanocomposite, polymer matrix and the polymer/particle interphase in the transverse state ($\theta = 0^\circ$) respectively. $A_c = 1$,

$A = k_2^2$ and $A_{mT} = 1 - A$ are the cross-section area of the nanocomposite, the interphase and the polymer matrix respectively.

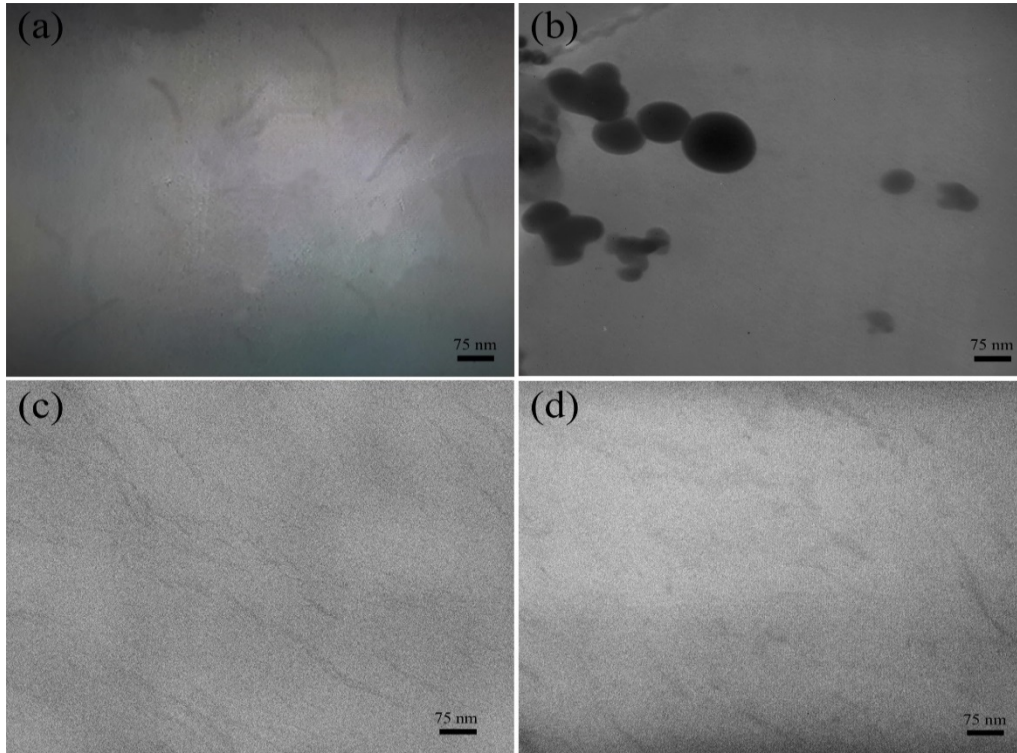


Figure 1. TEM images of (a) PS/CNT, (b) PS/SI, (c) and (d) PS/GO nanocomposites samples.

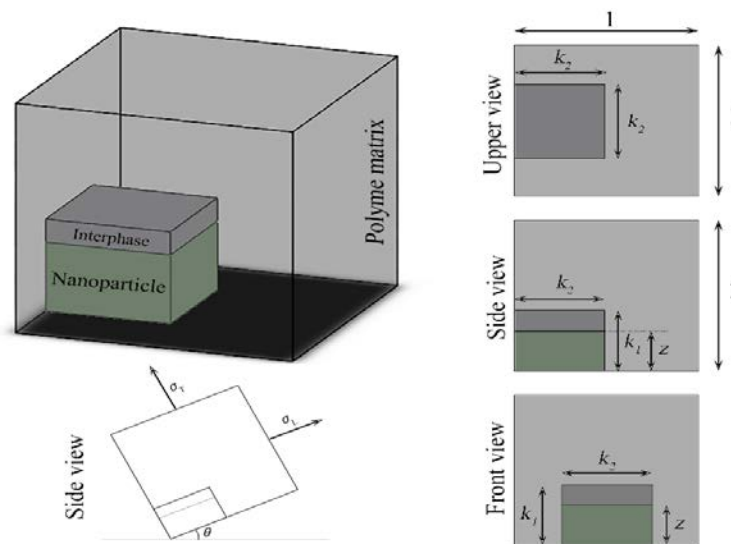


Figure 2. The structure of the model for nanocomposites containing platelet nanoparticles.

Though, at $\theta = 90^\circ$ it is essential to rearrange Equation (2) in order to describe the system performance against the longitudinal

force:

$$\sigma_{cL}A_c = \sigma_{mL}A_{mL} + \sigma_{iL}A \quad (3)$$

where, σ_{cL} , σ_{mL} and σ_{iL} are the tensile strength of nanocomposite, the polymer matrix and the polymer/particle interphase in the longitudinal state ($\theta = 90^\circ$) respectively, and $A_{mL} = A_{mT}$. Considering the polymer matrix as a homogenous material, it is possible to assume $\sigma_{mT} = \sigma_{mL}$ however due to the very small size of the interphase region and its role in transferring the shear force to the nanoparticle, it is impossible to use the same assumptions. According to the Von Mises criterion, $\sigma_{iL} = 0.577\sigma_{iT}$ if the polymer/particle interphase is considered homogeneous which is quite acceptable considering the very small size of the region. Though, it should be mentioned that the

properties of the polymer/particle interphase vary with the distance from the surface of the nanoparticle in the nanoscale [22, 41, 42]. Using Equations (2) and (3), it is possible to calculate the tensile strength of polymer nanocomposites considering the random orientation of the nanoparticles:

$$\sigma_c = \frac{\int_0^{90-\alpha} \sigma_{c1}(\theta) d\theta + \int_{90-\alpha}^{90} \sigma_{c2}(\theta) d\theta + \sigma_v}{\int_0^{90} d\theta} \quad (4)$$

where, $\sigma_v = \sqrt{\sigma_{cL}^2 + \sigma_{cT}^2}$, $\alpha = \text{Arctan}\left(\frac{\sigma_{cT}}{\sigma_{cL}}\right)$

and the other parameters are presented in Table 1.

Table 1
The parameters of Equation 4.

Parameter	1	2
$\sigma_c(\theta)$	$\sigma_v \sin(\lambda_1) - m_1 \sigma_v \cos(\lambda_1)$	$m_2 \sigma_v \sin(\lambda_2) - \sigma_v \cos(\lambda_2)$
λ	$(\alpha + \theta)$	$(\alpha + \theta - 90)$
m	$\frac{\sigma_v \sin(\lambda_1) - \sigma_{cT} \sin(\pi/2 - \theta)}{\sigma_v \cos(\lambda_1) - \sigma_{cT} \cos(\pi/2 - \theta)}$	$\frac{\sigma_v \cos(\lambda_2) - \sigma_{cL} \sin(\theta)}{-\sigma_v \sin(\lambda_2) - \sigma_{cL} \cos(\theta)}$

3.2. Nanocomposites containing cylindrical nanoparticles

The schematic of the model structure is presented in Figure 3. The model parameters can be determined using the following equations based on the quantitative values of the actual system:

$$\begin{cases} \frac{\pi z^2}{4} k_2 = \phi'_d \\ \frac{\pi k_1^2}{4} k_2 = \phi'_d + t(1 - \chi) A_T \\ 1 - \frac{\pi k_1^2}{4} k_2 = \phi'_m \end{cases} \quad (5)$$

The transversely and longitudinally tensile strengths of the system can be determined using Equations (2) and (3) respectively, considering $A_c = 1$, $A = k_1 k_2$, $A_{mT} = 1 - A$ and $A_{mL} = 1 - \pi k_1^2 / 4$. Consequently, the tensile strength of the system based on the random orientation of the nanoparticles is calculable using Equation (4).

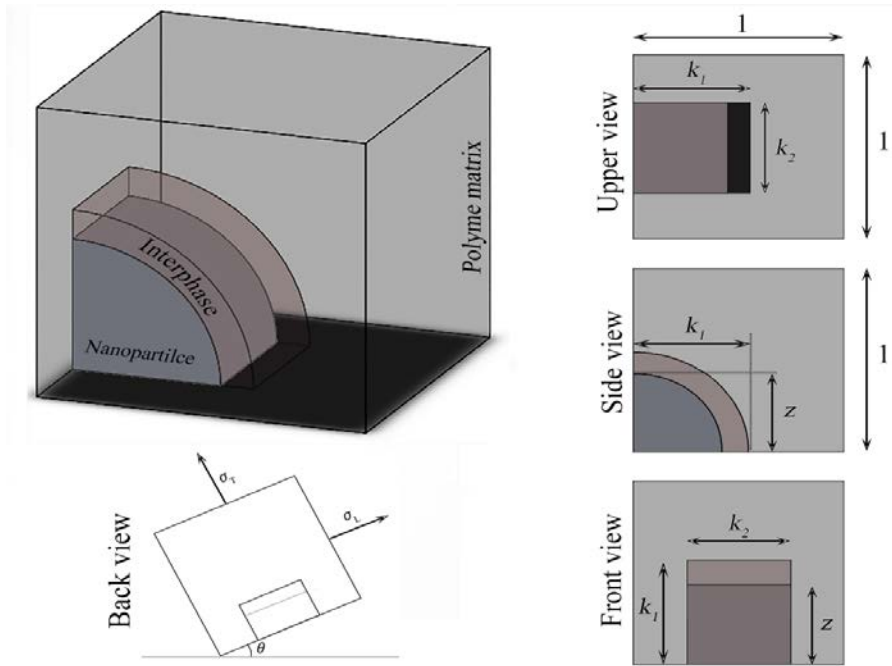


Figure 3. The structure of the model for nanocomposites containing cylindrical nanoparticles.

3.3. Nanocomposites containing spherical nanoparticles

The model structure of the nanocomposites containing spherical nanoparticles is presented in Figure 4. As it is mentioned before, the random orientation does not affect the performance of the spherical nanoparticles in such systems and therefore, the tensile strength can be simply determined using Equation (6):

$$\sigma_c A_c = \sigma_m A_m + \sigma_i A \quad (6)$$

where, $A = \pi k^2/2$ and $A_m = 1 - A$. Furthermore, the model parameter can be defined as follows:

$$\begin{cases} \phi'_d = \frac{\pi z^3}{3} \\ \frac{1}{3} \pi (k^3 - z^3) = \phi'_d (1 - \chi) A_T \end{cases} \quad (7)$$

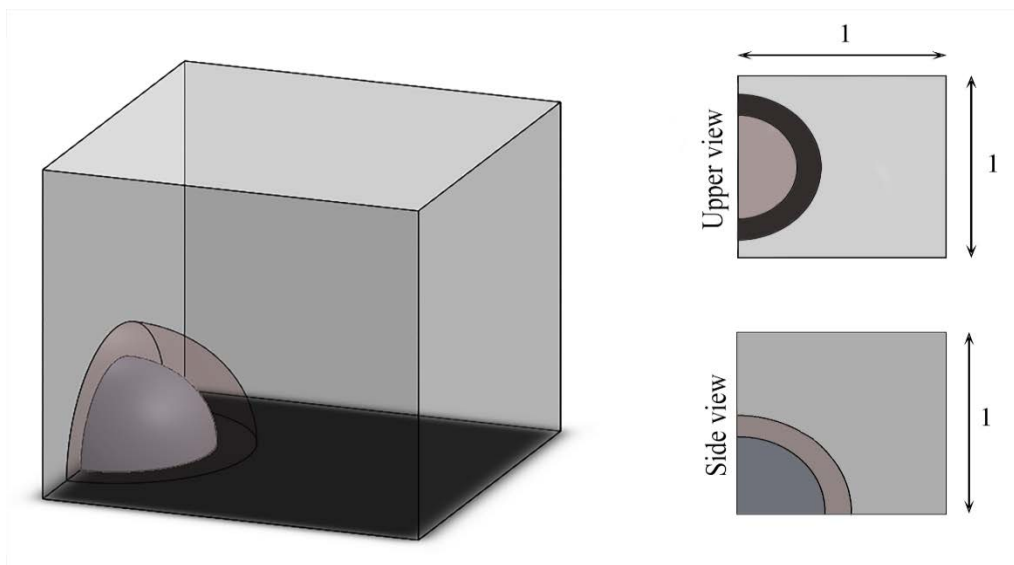


Figure 4. The structure of the model for nanocomposites containing spherical nanoparticles.

3.4. Consistency analysis

Evaluating the consistency of the model predictions with the experimental results requires the following steps to be accomplished:

(I): Interpreting the tensile strength and thickness of the polymer/particle interphase by coupling the model Equations and experimental results (at a low nanoparticle content). In this step, the interpretation should be performed at $\chi = 0$ which implies that there is no nanoparticle aggregation/agglomeration in the system.

(II): Defining parameter χ by coupling the experimental results of the samples containing different amounts of nanoparticles with the model equations. In the case of nanocomposites with a low nanoparticle content (< 0.5 vol. %) it was found that considering $\chi = 0.07$ % results in a prediction error of 7-9 %.

(III): Calculating prediction error using the relative error formula.

It should be noted that the prediction error

values are very important in evaluating the consistency of the model with the actual results and therefore, they should be precisely defined.

4. Results and discussion

The tensile test results for the prepared nanocomposites samples of different compositions are presented in Table 2. In our previous work, it was proved that the aggregation/agglomeration of nanoparticles was an inevitable phenomenon even at the low amounts of nanoparticle and directly affected the mechanical properties of the nanocomposite systems [43]. The effect of this phenomenon is quite observable in Table 2 since the increasing trend of the tensile strength changes to the decreasing one according to the amount of the nanoparticles. It is notable that, the effect of the aggregation/agglomeration of nanoparticles on the characteristics of the interphase region is neglected in the present model in order to prevent further complexity.

Table 2

The results of the tensile test for the different prepared samples.

Nanoparticle content (vol. %)	Tensile strength (Mpa)		
	PS/SI	PS/CNT	PS/GO
0.1	35.81±0.36	37.21±0.29	36.12±0.11
0.2	36.46±0.32	38.15±0.22	36.89±0.14
0.3	37.17±0.25	39.01±0.18	37.01±0.21
0.4	37.95±0.33	40.62±0.11	39.72±0.15
Matrix tensile strength = 34.91±2.8 (Mpa)			

Considering low values for the parameter χ at very low amounts of nanoparticles (e. g. 0.1 vol. %) [43], the thickness and tensile strength of the interphase region can be determined using the experimental data and the model equations for $\chi = 0$ (Table 3). As it is mentioned before, the tensile strength of the

interphase region is different in transverse and longitudinal directions ($\sigma_{iL} = 0.577\sigma_{iT}$) which implies the importance of the random orientation of the nanoparticles being considered in the modeling procedure. Accordingly, the parameter θ should be essentially considered in the range of $0^\circ - 90^\circ$.

Table 3

The thickness and tensile strength of the polymer/particle interphase interpreted from experimental results of samples containing 0.1 vol. % of nanoparticles.

	Thickness (t), (nm)	Tensile strength (σ_{IT}/σ_m)
PS/SI	1.89±0.13	4.21
PS/CNT	2.12±0.17	5.68
PS/GO	1.74±0.1	4.85

Considering independent and constant characteristics of the interphase region (Table 3) the model predictions for fully dispersed nanocomposites ($\chi = 0$) were compared with the actual experimental data in order to emphasize the drastic effects of the aggregation/agglomeration of nanoparticles on the tensile strength of nanocomposite

systems (Table 4). According to Table 4, the prediction error significantly increases with the volume fraction of nanoparticles which shows that the varying trend of the tensile strength, as a function of the amount of the nanoparticles, is significantly affected by parameter χ [44, 45]. This was also discussed based on the results of Table 2.

Table 4

The model predictions considering $\chi = 0$.

Nanoparticle content (vol. %)	Model predictions (Mpa)					
	PS/SI		PS/CNT		PS/GO	
	σ_c	Error (%)	σ_c	Error (%)	σ_c	Error (%)
0.1	36.96	3.2	38.28	2.9	36.98	2.4
0.2	38.21	4.8	39.33	3.09	37.72	2.2
0.3	39.04	5.03	41.24	5.7	39.26	6
0.4	41.22	8.61	45.52	12.06	40.61	10.6

Table 5 represents the aggregation/agglomeration percentage for each sample defined by coupling the experimental data and the model Equations. As it clear, considering the same sample preparation conditions, parameter χ increases with the volume fraction of nanoparticles even in the nanocomposites containing very low amounts of nanoparticles, as reported in our previous works [8, 19, 43]. It was found

that considering $\chi = 0.07$ % results in a prediction error of 7-9 % for the nanocomposites containing low volume fractions of nanoparticles (< 0.5 vol. %) which is quite acceptable. Though, the aggregation/agglomeration percentage and the resulted prediction errors should be calculated, as described, for the samples with the nanoparticle amount out of the studied range.

Table 5

The value of χ for the prepared samples.

Nanoparticle content (vol. %)	χ (%)		
	PS/SI	PS/CNT	PS/GO
0.1	0.012	0.008	0.006
0.2	0.036	0.031	0.022
0.3	0.059	0.062	0.074
0.4	0.087	0.113	0.091

Figure 5 illustrates the analysis results based on Tables 2-5. As it is clear, the model predictions trend is significantly affected by χ value since applying the corresponding χ of each sample in the modeling procedure (Table 5) leads to a less prediction error. On the other hand, considering χ as a constant ($\chi =$

0.07 %) can also provide good predictions and simplify the modeling procedure. Accordingly, $\chi = 0.07$ % can be considered as an optimum value for the nanocomposite systems containing low amount of nanoparticles (< 0.05 vol. %).

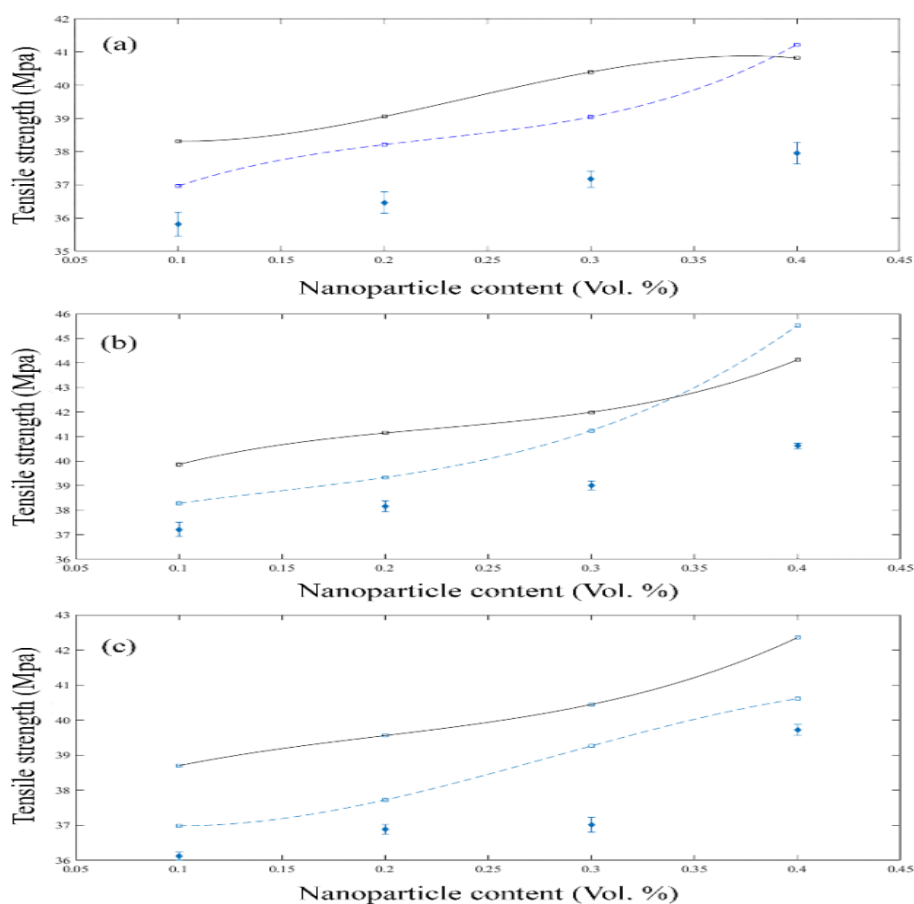


Figure 5. The model prediction results for (a) PS/SI, (b) PS/CNT and (c) PS/GO nanocomposites based on the result of Tables 2-5. (♦) Experimental data, (---) model predictions according to χ values presented in Table 5, (—) model prediction based on $\chi = 0.07$ %.

Moreover, in order to investigate the practicality of the model at the high amounts of nanoparticles (> 1 % vol.), the model predictions were also compared to some data from the literature (Table 6) [46].

According to Table 6, the prediction error relatively increases at high amounts of nanoparticles however, in an acceptable range (< 10 %). It should be noted that the tensile strength of PP/SiO₂ nanocomposite decreases

at a specific weight fraction (2 wt %) which can be attributed to the aggregation/agglomeration and reinforcing effects of nanoparticles [47-50]. This phenomenon can be seen in almost all nanocomposite which causes the tensile strength of the system to decrease even below the tensile strength of the polymer matrix [38, 47, 51, 52]. Accordingly, the presented model needs to be capable of

predicting the tensile strength of the nanocomposite even after the mentioned point which is perfectly done by the presented model. Considering $\chi = 0.07\%$ resulted in a prediction error of 7-9 % for Epoxy/SWNT nanocomposite, as reported for the prepared nanocomposite samples, while this value was 15-18 % for PP/SiO₂ nanocomposite.

Therefore, in the case of nanocomposites containing high contents of nanoparticles, it is better to exclusively evaluate the parameter χ for each sample. Figure 6 illustrates the modeling results for PP/SiO₂ and Epoxy/SWNT nanocomposites based on the presented data in Table 6.

Table 6

The evaluation of PP/SiO₂ and Epoxy/SWNT nanocomposites. Data are collected from reference No. [46].

Nanoparticle content (wt. %)	Tensile strength (Mpa)	Thickness (t), (nm)	Tensile strength of the interphase (σ_{IT}/σ_m)	χ (%)	Model predictions (Mpa)	Error (%)
PP/SiO ₂						
1	37.5			0.46	40.61	8.3
2	38.1	2.42	5.17	0.89	41.6	9.2
3	37.9			1.53	40.89	7.9
Epoxy/SWNT						
0.05	65.84			0.006	67.94	3.2
0.1	66.34	1.73	3.88	0.013	68.72	3.6
0.3	67.28			0.048	70.03	4.1

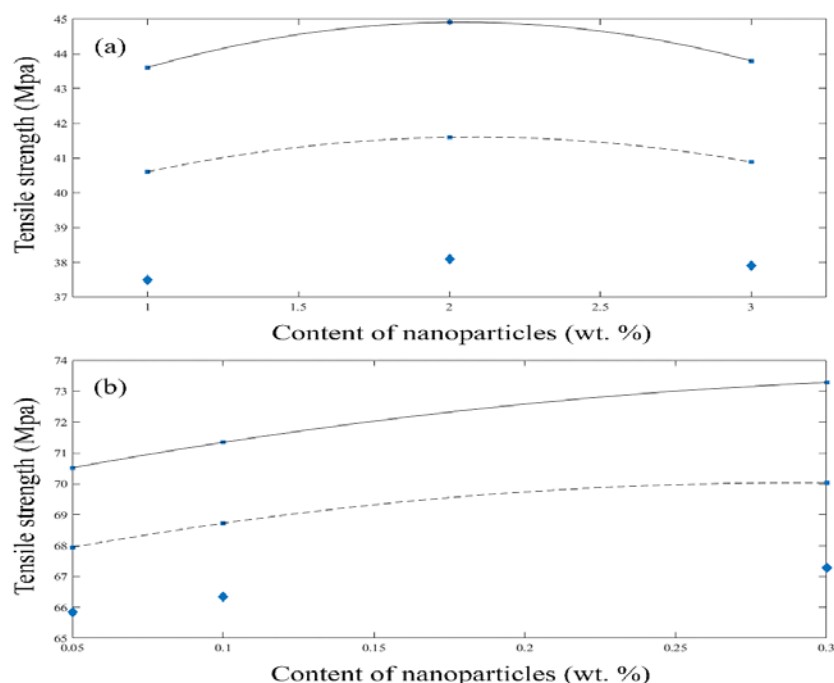


Figure 6. The model prediction results for (a) PP/SiO₂ and (b) Epoxy/SWNT based on the result of Tables 6. (♦) Experimental data, (---) model predictions according to χ values presented in Table 5, (—) model prediction base on $\chi = 0.07\%$.

5. Conclusions

A model was proposed for predicting the tensile strength of the nanoparticles based on considering the aggregation/agglomeration, the random orientation of nanoparticles and also the effects of the polymer/particle interphase. It was proved that the aggregation/agglomeration of the nanoparticles is an inevitable phenomenon and should be definitely considered in the modeling procedure. Furthermore, as illustrated in Figure 1, the random orientation of platelet and cylindrical nanoparticles was considered a determinative factor in the model. Furthermore, the presented model made it possible to define the characteristics of the polymer/particle region (the thickness and tensile strength) which can be mentioned as one of its advantages compared to other similar models. The comparison between the model predictions and the tensile test results revealed that considering $\chi = 0.07\%$ at low amounts of nanoparticles (< 0.5 vol. %) results in an acceptable prediction error (7-9 %) for different shapes of nanoparticles. It was also proved that the model was capable of predicting the tensile strength of nanocomposites containing high amount of nanoparticles with predicting error of less than 10 %.

References

- [1] Paul, D. R. and Robeson, L. M., "Polymer nanotechnology: Nanocomposites", *Polymer*, **49** (15), 3187 (2008).
- [2] Ramesan, M. T. and Suhailath, K., 13- Role of nanoparticles on polymer composites, in Micro and nano fibrillar composites (MFCs and NFCs) from polymer blends, Mishra, R. K., Thomas, S. and Kalarikkal, N. Editors, Woodhead Publishing, p. 301 (2017).
- [3] Nasir, A., Kausar, A. and Younus, A., "A review on preparation, properties and applications of polymeric nanoparticle-based materials", *Polymer-Plastics Technology and Engineering*, **54** (4), 325 (2015).
- [4] Li, S., Meng Lin, M., Toprak, M. S., Kim, D. K. and Muhammed, M., "Nanocomposites of polymer and inorganic nanoparticles for optical and magnetic applications", *Nano Reviews*, **1** (1), (2010). (<https://doi.org/10.3402/nano.v1i0.5214>).
- [5] Sadasivuni, K. K., Rattan, S., Waseem, S., Brahme, S. K., Kondawar, S. B., Ghosh, S., Das, A. P., Chakraborty, P. K., Adhikari, J., Saha, P. and Mazumdar, P., Silver nanoparticles and its polymer nanocomposites-synthesis, optimization, biomedical usage, and its various applications, in Polymer nanocomposites in biomedical engineering, Sadasivuni, K. K. et al., Editors, Springer International Publishing, Cham, p. 331 (2019).
- [6] Karak, N., Nanomaterials and polymer nanocomposites: Raw materials to applications, Elsevier Science, (2018).
- [7] Pielichowski, K. and Majka, T. M., Polymer composites with functionalized nanoparticles: Synthesis, properties, and applications, Elsevier Science, (2018).
- [8] Sharifzadeh, E., Salami-Kalajahi, M., Hosseini, M. S. and Aghjeh, M. K. R., "Synthesis of silica Janus nanoparticles by buoyancy effect-induced desymmetrization process and their placement at the PS/PMMA interface", *Colloid. Polym. Sci.*, **295** (1), 25 (2017).
- [9] Crosby, A. J. and Lee, J. Y., "Polymer nanocomposites: The "Nano" effect on

- mechanical properties”, *Polymer Reviews*, **47** (2), 217 (2007).
- [10] Zaragoza, J., Fukuoka, S., Kraus, M., Thomin, J. and Asuri, P., “Exploring the role of nanoparticles in enhancing mechanical properties of hydrogel nanocomposites”, *Nanomaterials (Basel, Switzerland)*, **8** (11), 882 (2018).
- [11] Sallal, H. A., Abdul-Hamead, A. A. and Othman, F. M., “Effect of nano powder ($\text{Al}_2\text{O}_3\text{-CaO}$) addition on the mechanical properties of the polymer blend matrix composite”, *Defence Technology*, (2019).
- [12] Ashraf, M. A., Peng, W., Zare, Y. and Rhee, K. Y., “Effects of size and aggregation/agglomeration of nanoparticles on the interfacial/interphase properties and tensile strength of polymer nanocomposites”, *Nanoscale Research Letters*, **13** (1), 214 (2018).
- [13] Zhao, W., Li, T., Li, Y., O'Brien, D. J., Terrones, M., Wei, B., Suhr, J. and Lucas Lu, X., “Mechanical properties of nanocomposites reinforced by carbon nanotube sponges”, *Journal of Materiomics*, **4** (2), 157 (2018).
- [14] Sergueeva, A. V., Hulbert, D. M., Mara, N. A. and Mukherjee, A. K., Chapter 3- Mechanical properties of nanocomposite materials, in *Frontiers of nanoscience*, Wilde, G. Editor, Elsevier, p. 127 (2009).
- [15] Liu, Y., Wu, H. and Chen, G., “Enhanced mechanical properties of nanocomposites at low graphene content based on in situ ball milling”, *Polym. Compos.*, **37** (4), 1190 (2016).
- [16] Mechanical properties of polymer nanocomposites, in *Fundamentals, properties, and applications of polymer nanocomposites*, Koo, J. H. Editor, Cambridge University Press, Cambridge, p. 273 (2016).
- [17] Hore, M. J. A., “Polymers on nanoparticles: Structure & dynamics”, *Soft Matter*, **15** (6), 1120 (2019).
- [18] Hyun, H., Park, J., Willis, K., Park, J. E., Lyle, L. T., Lee, W. and Yeo, Y., “Surface modification of polymer nanoparticles with native albumin for enhancing drug delivery to solid tumors”, *Biomaterials*, **180**, 206 (2018).
- [19] Sharifzadeh, E., “Modeling of the mechanical properties of blend based polymer nanocomposites considering the effects of Janus nanoparticles on polymer/polymer interface”, *Chin. J. Polym. Sci.*, **37** (2), 164 (2019).
- [20] Jesson, D. A. and Watts, J. F., “The interface and interphase in polymer matrix composites: Effect on mechanical properties and methods for identification”, *Polymer Reviews*, **52** (3), 321 (2012).
- [21] Zare, Y., “Modeling the strength and thickness of the interphase in polymer nanocomposite reinforced with spherical nanoparticles by a coupling methodology”, *J. Colloid Interface Sci.*, **465**, 342 (2016).
- [22] De Gennes, P. G., “Scaling theory of polymer adsorption”, *J. Phys. France*, **37** (12), 1445 (1976).
- [23] Sharifzadeh, E., Ghasemi, I., Karrabi, M. and Azizi, H., “A new approach in modeling of mechanical properties of binary phase polymeric blends”, *Iran. Polym. J.*, **23** (7), 525 (2014).
- [24] Sharifzadeh, E., Ghasemi, I., Karrabi, M. and Azizi, H., “A new approach in modeling of mechanical properties of nanocomposites: Effect of interface region and random orientation”, *Iran. Polym. J.*, **23** (11), 835 (2014).

- [25] Ciprari, D., Jacob, K. and Tannenbaum, R., "Characterization of polymer nanocomposite interphase and its impact on mechanical properties", *Macromolecules*, **39** (19), 6565 (2006).
- [26] Zakaria, A. Z. and Shelesh-Nezhad, K., "The effects of interphase and interface characteristics on the tensile behaviour of POM/CaCO₃ nanocomposites", *Nanomaterials and Nanotechnology*, **4**, 17 (2014).
- [27] Seiler, J. and Kindersberger, J., "Insight into the interphase in polymer nanocomposites", *IEEE Transactions on Dielectrics and Electrical Insulation*, **21** (2), 537 (2014).
- [28] Sharifzadeh, E., Ghasemi, I. and Safajou-Jahankhanemlou, M., "Modulus prediction of binary phase polymeric blends using symmetrical approximation systems as a new approach", *Iran. Polym. J.*, **24** (9), 735 (2015).
- [29] Sharifzadeh, E., Ghasemi, I. and Qarebagh, A. N., "Modeling of blend-based polymer nanocomposites using a knotted approximation of Young's modulus", *Iran. Polym. J.*, **24** (12), 1039 (2015).
- [30] Blattmann, C. O. and Pratsinis, S. E., "Nanoparticle filler content and shape in polymer nanocomposites", *KONA Powder and Particle Journal*, **36**, 3 (2019).
- [31] Sharifzadeh, E., Salami-Kalajahi, M., Salami Hosseini, M., Razavi Aghjeh, M. K., Najafi, S., Jannati, R. and Hatef, Z., "Defining the characteristics of spherical Janus particles by investigating the behavior of their corresponding particles at the oil/water interface in a Pickering emulsion", *J. Dispersion Sci. Technol.*, **38** (7), 985 (2017).
- [32] Zare, Y., "Study of nanoparticles aggregation/agglomeration in polymer particulate nanocomposites by mechanical properties", *Composites Part A: Applied Science and Manufacturing*, **84**, 158 (2016).
- [33] Zare, Y., "Modeling the yield strength of polymer nanocomposites based upon nanoparticle agglomeration and polymer-filler interphase", *J. Colloid Interface Sci.*, **467**, 165 (2016).
- [34] Mittal, V., Modeling and prediction of polymer nanocomposite properties, Wiley, (2012).
- [35] Zare, Y., "The roles of nanoparticles accumulation and interphase properties in properties of polymer particulate nanocomposites by a multi-step methodology", *Composites Part A: Applied Science and Manufacturing*, **91**, 127 (2016).
- [36] Zhu, L. and Narh, K. A., "Numerical simulation of the tensile modulus of nanoclay-filled polymer composites", *J. Polym. Sci., Part B: Polym. Phys.*, **42** (12), 2391 (2004).
- [37] Bataille, P., Boissé, S. and Schreiber, H. P., "Mechanical properties and permeability of polypropylene and poly(ethylene terephthalate) mixtures", *Polym. Eng. Sci.*, **27** (9), 622 (1987).
- [38] Sharifzadeh, E., "Modeling of the tensile strength of immiscible binary polymer blends considering the effects of polymer/polymer interface and morphological variation", *Chin. J. Polym. Sci.*, **37**, 1176 (2019).
- [39] Zare, Y., "Modeling approach for tensile strength of interphase layers in polymer nanocomposites", *J. Colloid Interface Sci.*, **471**, 89 (2016).
- [40] Sharifzadeh, E., Salami-Kalajahi, M.,

- Salami Hosseini, M., Razavi Aghjeh, M. K., "A temperature-controlled method to produce Janus nanoparticles using high internal interface systems: Experimental and theoretical approaches", *Colloids and surfaces. A*, **506**, 56 (2016).
- [41] Surhone, L. M., Timpledon, M. T. and Marseken, S. F., Von mises yield criterion, VDM Publishing, (2010).
- [42] Leckie, F. A. and Bello, D. J., Strength and stiffness of engineering systems, Springer US, (2009).
- [43] Sharifzadeh, E. and Amiri, Y., "The effects of the arrangement of Janus nanoparticles on the tensile strength of blend-based polymer nanocomposites", *Polym. Compos.*, (2020). (<https://doi.org/10.1002/pc.25645>).
- [44] Haghi, A. K., Update on nanofillers in nanocomposites: From introduction to application, Smithers Information Limited, (2013).
- [45] Kumar, C. S. S. R., Nanocomposites, Wiley, (2010).
- [46] Tjong, S. C., "Structural and mechanical properties of polymer nanocomposites", *Materials Science and Engineering: R: Reports*, **53** (3), 73 (2006).
- [47] Zare, Y. and Rhee, K. Y., "Evaluation of the tensile strength in carbon nanotube-reinforced nanocomposites using the expanded Takayanagi model", *JOM*, **71** (11), 3980 (2019).
- [48] Salam, H. and Dong, Y., "Theoretical modelling analysis on tensile properties of bioepoxy/clay nanocomposites using epoxidised soybean oils", *Journal of Nanomaterials*, **2019**, 4074869 (2019).
- [49] Ghasemi, F. A., Niyaraki, M. N., Ghasemi, I. and Daneshpayeh, S., "Predicting the tensile strength and elongation at break of PP/graphene/glass fiber/EPDM nanocomposites using response surface methodology", *Mechanics of Advanced Materials and Structures*, **1** (2019).
- [50] Harito, C., Bavykin, D. V., Yulianto, B., Dipojono, H. K. and Walsh, F. C., "Polymer nanocomposites having a high filler content: Synthesis, structures, properties, and applications", *Nanoscale*, **11** (11), 4653 (2019).
- [51] Khan, I., Saeed, K. and Khan, I., "Nanoparticles: Properties, applications and toxicities", *Arabian Journal of Chemistry*, **12** (7), 908 (2019).
- [52] Zare, Y. and Rhee, K. Y., "A simulation work for the influences of aggregation/agglomeration of clay layers on the tensile properties of nanocomposites", *JOM*, **71** (11), 3989 (2019).