Iranian Journal of Chemical Engineering

Research Note

Investigating the Effects of Hollow Graphene Oxide Nanoparticles on the Thermal/Mechanical Properties of Polymer Nanocomposites: Experimental, Analytical and Simulation Approaches

F. Ader [1,2], E. Sharifzadeh [1,2*]

[1] *Department of Chemical Engineering, Faculty of Petroleum and Chemical Engineering, Razi University, Kermanshah, Iran*
[2] *Polymer Research Division, Advanced Chemical Engineering Research Center, Razi University, Kermanshah, Iran*

ARTICLE INFO	ABSTRACT
	In this study, the main purpose has been to investigate the behavior of the nanoparticles with different structures and similar based materials in polymer nanocomposites. To this end, different samples, containing PS as the matrix, and layered graphene oxide (GO) and/or hollow graphene oxide nanoparticles (HGO), were prepared via the melt mixing process and were subjected to heat conduction and tensile tests. To evaluate all features of the interaction between the polymer phase and the nanoparticles, a thermal/mechanical analytical model was proposed and the results were used to simulate the behavior of specific geometrical structures, corresponding to the real samples, under different thermal/mechanical conditions. The results showed good agreement between the obtained experimental data and simulation/analytical model interpretations. In addition, it was found that the HGO nanoparticle had such a good performance in enhancing the thermal and mechanical properties of the nanocomposite, due to its unique structure.

1. Introduction

The addition of different types of nanoparticles to a polymer matrix has always been considered as a good choice to enhance the physical/mechanical properties of the system [1-3]. This strategy is also helpful in the case of polymer blends, consisting of two or more polymer phases, in which the performance and localization of the nanoparticles are considered as very effective parameters to control the final characteristics of the products [4-8]. Unlike that of single-phase polymer systems, the polymer/polymer interface plays a determinative role in

---

* Corresponding author: e.sharifzadeh@razi.ac.ir (E. Sharifzadeh)

defining the response mechanism of the system against the exerted driving forces (e. g. stress, thermal, etc.) [6, 8-10]. It is proved that nanoparticles can drastically improve the mechanical/physical characteristics of polymers and polymer blends however, it is essential to have the nanoparticles compatible with the polymer phase(s) [2, 11]. Properties such as the tensile modulus, tensile strength, thermal conductivity and viscosity are the most investigated subjects in recent decades since they provide valuable information about the processibility and the final performance of the products [12, 13].

There are many approaches of which the purpose is to introduce a practical method to better comprehend polymer nanocomposites using the advantages of both experimental and modeling methods [14, 15]. Indeed, the experimental methods cannot always provide comprehensive information about all aspects of the interaction between nanoparticles and the polymer phase since many parameters are not experimentally measurable [3, 9, 11, 16]. The physical/mechanical properties of the polymer/particle interphase region (e. g. the thickness, tensile strength and modulus, thermal conductivity, etc.), aggregation/agglomeration factor, the effect of the type, shape and structure of the nanoparticle on their performance in the system, etc. are of the most important parameters, which can be interpreted by coupling efficient mathematical models with related experimental results [5, 11, 17]. Meanwhile, simulation is also another practical method to design a nanocomposite system according to the available data set and compare it with the actual system [1]. This helps to define the details about the differences and similarities between the analytical based and actual systems, and better improve the evaluation strategies.

As mentioned, the type and surface chemistry of the nanoparticles and their compatibility with the system significantly affect the polymer nanocomposites [18, 19]. For instance, adding apolar nanoparticles to a polar polymer phase leads to a major aggregation/agglomeration and the decrement of the physical/mechanical properties of the nanocomposite [19]. On the contrary, enhancing the compatibility of the nanoparticle with the polymer matrix facilitates their dispersion/distribution and increases their corporation with the system against the exerted driving force. Generally, the compatible nanoparticles attract polymer chains onto their surface, which, according to the self-similar carpet and selective physisorption theories, cause the formation of the polymer/particle interphase region [1, 11]. The characteristics of this region depend on the properties of the polymer phase, surface chemistry of the nanoparticles, processing parameters, etc. among which, the type of superficial groups has been introduced as the most effective parameter [20]. This has persuaded the investigators to propose different surface modification processes, using different agents, to produce the nanoparticles compatible with the symmetric or asymmetric surface chemistry [21, 22]. Janus nanoparticles, known as asymmetric nanoparticles, are capable to be simultaneously compatible with two phases which make these types of nanoparticles a remarkable choice to improve the physical/mechanical properties of the blend-based polymer nanocomposites [23-25]. There are many methods to produce such nanoparticles among which the desymmetrization process provides the highest qualitative/quantitative efficiencies

[26-28]. Moreover, it is proved that Janus nanoparticles are capable of controlling the polymer/polymer interface in immiscible blends, which substantially alters the properties of the system [4, 5, 16].

Also, the structure and the type of nanoparticles have a substantial effect on the characteristics of the nanocomposites. For example, carbon-based nanoparticles (graphene, graphene oxide (GO), carbon nanotube, etc.) can improve both thermal and mechanical properties of the polymer phase(s), while silica nanoparticles are not good heat conductors [1, 16]. Also, the random orientation is meaningless in the case of spherical nanoparticles, while it is very important to evaluate the orientation factor for cylindrical and plate shape nanoparticles [30]. It has been proved that hollow structured nanoparticles have very interesting characteristics, which become more unique while being applied to polymers [23]. We have previously proposed a developed hydrothermal method to synthesize micro and nano-sized hollow graphene oxide nanoparticles, which were used as simple and Janus particles in single and double phase polymer systems [16, 23].

Accordingly, in this study an efficient analytical model has been designed considering the effects of the characteristics of the polymer/particle interphase and the aggregation/agglomeration factor to evaluate the physical/mechanical properties of the polymer nanocomposites containing hollow graphene oxide (HGO) nanoparticles. The main purpose was to reveal the differences between the performance of the layered and hollow graphene oxide nanoparticles in polymer nanocomposites, due to their different structures. The results of the model were compared with the data obtained from the performed tensile and heat conduction tests on the prepared Polystyrene (PS) samples, via melt mixing, containing different amounts of synthesized HGO or graphene oxide (GO) nanoparticles (1-4 Vol. %). Also, the systems were simulated using the ABAQUS software to investigate the mechanism of the impact of HGO nanoparticles on the thermal/mechanical characteristics of the nanocomposites. According to the experimental and theoretical results, the HGO nanoparticles better enhanced the thermal/mechanical properties of the nanocomposite samples which, considering the same base materials of HGO and GO nanoparticles, was attributed to their effective structures.

2. Modeling background
2.1. Analytical modeling based on the equivalent box model method

As mentioned, there are many components in a polymer nanocomposite and each has a specific role in the response mechanism of the system against the exerted driving force. Accordingly, it was important to design a geometrical structure, corresponding to the real system and by which it was possible to discriminate each component and investigate its performance solely. We have previously proposed different geometrical structures in the case of polymer nanocomposites containing spherical nanoparticles [2, 7, 11]. However, in the case of the hollow graphene oxide (HGO) nanoparticles, there was a significant difference due to their unique structure [16, 23]. Figure 1(a) demonstrates the geometrical structure, in 3D and 2D, corresponding to the nanocomposite systems containing HGO nanoparticles. As it is clear, the geometrical structure consists of a hollow component and its surrounding polymer

matrix, is indeed a hypothetical pattern of the system. It was also considered that the hollow space of the nanoparticles was occupied by air and the characteristics of the walls were similar to those of the graphene layers. Consequently, it was possible to define r_o, r_i and z using Equations (1), (2) and (3) respectively (Figure 1(b)):

$$r_o = \sqrt[3]{\frac{3w_n(1-\mu)}{\rho_n 4\pi}} \qquad (1)$$

$$r_i = N^{\frac{1}{3}}(r_a - t) \qquad (2)$$

$$z = \sqrt[3]{N\left((r_a + \tau)^3 - r_a^3\right) + r_o^3} \qquad (3)$$

where w_n and ρ_n denoted the weights of HGO nanoparticles in the sample and their apparent densities, N was the number of the HGO nanoparticles ($N = 3w_n / 4\pi\rho_n r_a^3$), μ was the aggregation/agglomeration factor, t was the thickness of the wall of HGO nanoparticles, τ denoted the thickness of the polymer/particle interphase, and r_a represented the actual radius of an individual nanoparticle obtained from the FE-SEM test. It should be noted that Equation 2 was derived based on neglecting the weight of the air inside the nanoparticles.
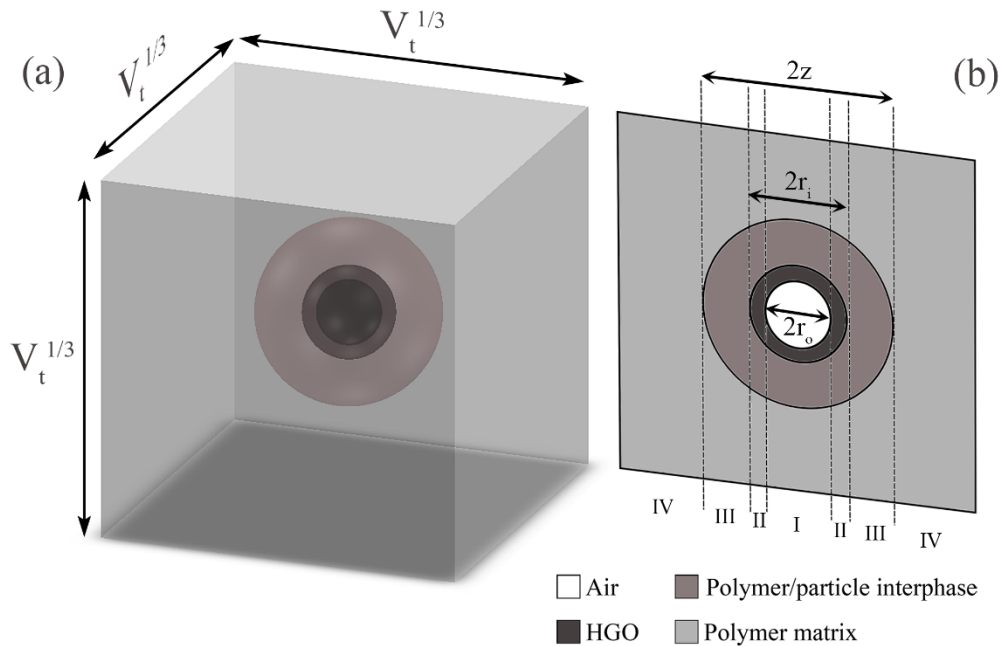

Figure 1. (a) 3D geometrical structure corresponding to the nanocomposite system containing HGO nanoparticles and (b) its series and parallel components.

According to Figure 1(b), the structure of nanocomposites was consisted of the hollow space, graphene oxide wall, polymer/particle interphase region and the polymer matrix, aligned as series and parallel components, according to the equivalent box model (EBM) [2, 4, 31] (Figure 2). In our previous works, we have proposed simple models to define the thermal conductivity of nanocomposite systems, using the advantages of EBM [11], according to which it was possible to formulate the thermal conductivity of the system (K_M) based on Figure 2:

$$K_M = \varphi_I K_I + \varphi_{II} K_{II} + \varphi_{III} K_{III} + \varphi_{IV} K_{IV} \qquad (4)$$

where, $\varphi_I = \pi r_i^2 / V_t^{\frac{2}{3}}$, $\varphi_{II} = \pi(r_o^2 - r_i^2)/V_t^{\frac{2}{3}}$,

$\varphi_{III} = \pi(z^2 - r_o^2)/V_t^{\frac{2}{3}}$, $\varphi_{IV} = 1 - (\varphi_I + \varphi_{II} + \varphi_{III})$.

V_t is the total volume of the sample, and $K_{IV} = K_m$. Also, K_I, K_{II} and K_{III} were calculated as follows:

$$K_I = \left(\frac{\varphi_{Air}}{K_{Air}} + \frac{\varphi_{wI}}{K_g} + \frac{\varphi_{iI}}{K_i} + \frac{\varphi_{mI}}{K_m} \right)^{-1} \tag{5}$$

$$K_{II} = \left(\frac{\varphi_{wII}}{K_g} + \frac{\varphi_{iII}}{K_i} + \frac{\varphi_{mII}}{K_m} \right)^{-1} \tag{6}$$

$$K_{III} = \left(\frac{\varphi_{iIII}}{K_i} + \frac{\varphi_{mIII}}{K_m} \right)^{-1} \tag{7}$$

where, K_{Air}, K_g, K_i, and K_m were the thermal conduction coefficients of air, graphene, the polymer/particle interphase region, and polymer matrix respectively. Also, $K_{IV} = K_m$.
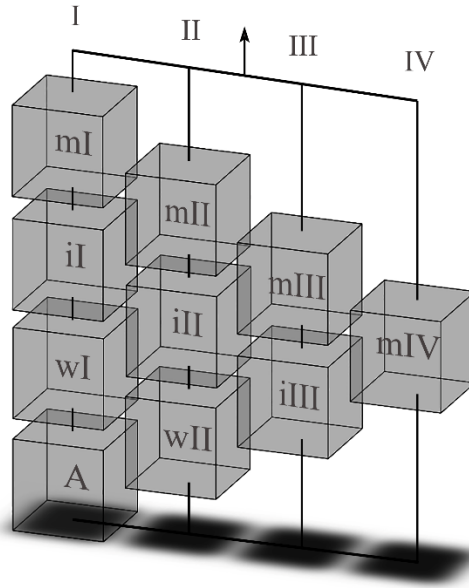

Figure 2. EBM model defining the interaction between the components of the nanocomposites system based on its representative geometrical structure, (Figure 1(b)).

Parameter φ, in each case, denoted the volume fraction of the components of EBM and was calculated as follows:

$$\varphi_{iIII} = \frac{1}{V_{III}} \left(\frac{4}{3} \pi \left(z^2 - r_o^2 \right)^{3/2} \right) \tag{8}$$

$$\varphi_{mIII} = \frac{1}{V_{III}} \left(\pi \left(z^2 - r_o^2 \right) V_t^{1/3} \right) - \varphi_{iIII} \tag{9}$$

$$\varphi_{wII} = \frac{1}{V_{II}} \left(\frac{4}{3} \pi \left(r_o^2 - r_i^2 \right)^{3/2} \right) \tag{10}$$

$$\varphi_{iII} = \frac{1}{V_{II}} \left(\frac{4}{3} \pi \left(z^2 - r_i^2 \right)^{3/2} \right) - \left(\varphi_{wII} + \varphi_{iIII} \right) \tag{11}$$

$$\varphi_{Air} = \frac{1}{V_I} \left(\frac{4}{3} \pi r_i^3 \right) \tag{12}$$

$$\varphi_{wI} = \frac{1}{V_I} \left(\frac{4}{3} \pi r_o^3 \right) - \left(\varphi_{wII} + \varphi_{Air} \right) \tag{13}$$

$$\varphi_{iI} = \frac{1}{V_I} \left(\frac{4}{3} \pi z^3 - \frac{4}{3} \pi \left(z^2 - r_i^2 \right)^{3/2} \right) - \left(\varphi_{Air} + \varphi_{wI} \right) \tag{14}$$

$$\varphi_{mII} = \frac{1}{V_{II}} \left(\pi \left(r_o^2 - r_i^2 \right) V_t^{1/3} \right) - \left(\varphi_{wII} + \varphi_{iII} \right) \tag{15}$$

$$\varphi_{mI} = \frac{1}{V_I} \left(\pi r_i^2 V_t^{1/3} \right) - \left(\varphi_{Air} + \varphi_{wI} + \varphi_{iI} \right) \tag{16}$$

where, V denoted the volume of each component, and $V_I = V_{Air} + V_{wI} + V_{iI} + V_{mI}$, $V_{II} = V_{wII} + V_{iII} + V_{mII}$, and $V_{III} = V_{iIII} + V_{mIII}$.

We have previously proved that the EBM can be considered as an efficient method for

evaluating the mechanical properties of polymer nanocomposites (e. g. the tensile modulus, tensile strength, yield strength, etc.) [2, 4]. Accordingly, substituting different thermal conduction coefficient parameters (K) of Equation (4) with their corresponding tensile modulus parameters (E) made it possible to develop the model in order to evaluate the tensile modulus of the nanocomposite system:

$$E_M = \varphi_I E_I + \varphi_{II} E_{II} + \varphi_{III} E_{III} + \varphi_{IV} E_{IV} \qquad (17)$$

It should be noted that all components of Equation (17) were the same as those introduced for Equation (4) except for the parameter K, which was substituted with E in the case of each component and $\varphi_{Air}/E_{Air} = 0$.

2.2. Simulation

The results obtained from the analytical model were used to compare the behavior of the nanocomposite samples containing HGO and GO nanoparticles via simulation. Figure 3 demonstrates the hypothetical thermal and mechanical conditions used in the process. It should be noted that both designed geometrical structures contained 2 Vol. % of the nanoparticles.
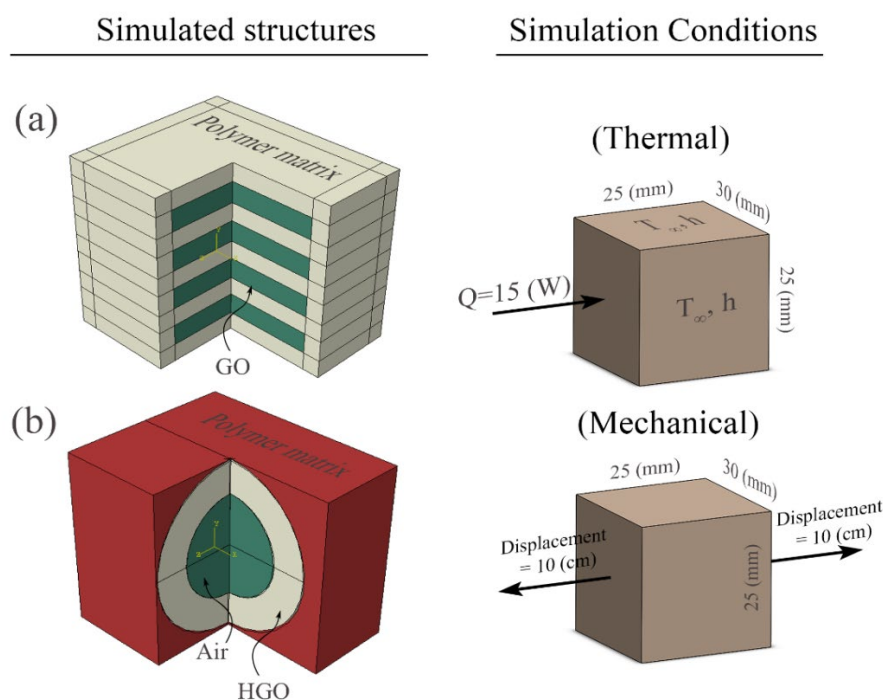

Figure 3. Hypothetical thermal and mechanical conditions used to simulate the behavior of the geometrical structures corresponding to the nanocomposite samples containing 2 Vol. % of (a) HGO and (b) GO nanoparticles.

3. Experimental
3.1. Materials
Graphene oxide (GO) and H_2SO_4 (> 99 %) were provided by Sigma Aldrich and Merck corporations respectively, and Polystyrene

(PS) (Grade 1160 GPPS, 1.04 $(g.mL^{-1})$) was used as received.

3.2. Sample preparation
The HGO nanoparticles were synthesized

according to our previously proposed hydrothermal method [16, 23]. The nanocomposite samples, containing 1-4 Vol. % of GO or HGO nanoparticles, were prepared via the melt mixing process in an internal mixer (Brabender Plasticorder W50EHT, Germany) at 200 °C and 60 rpm. The samples were then molded into suitable pieces using a hot-press device, at 200 °C and 30 bar, for tensile and heat conduction tests. It should be noted that the sample shape for the tensile test was in accordance with ISO-527 and the samples for the heat conduction test had a platelet shape with a diameter of 20 (mm) and a thickness of 2 (mm).

3.3. Characterization

A Zwick/Roell tensile testing machine (Z 010, Germany) was used to perform the tensile test, according to ISO-527, and the thermal conductivity of the nanocomposite samples was indicated using a heat conduction test unit (H940, P.A. Hilton, UK) with a heat flux of 4 $W.m^{-2}$. The apparent

density of HGO nanoparticles (ρ_n) was defined based on ISO 3923/1 (0.251 gr.mL^{-1}) and applied in Equation (18) to define the thickness of their wall (t) [23]:

$$t = r_a - \left(r_a^3 - \left(\frac{3\rho_a (2r_a)^3}{4\pi\rho_g} \right)^{1/3} \right) \qquad (18)$$

where ρ_g represented the density of the GO nanoparticles. The thickness of the wall of HGO nanoparticles was defined to be 2.47 (nm) based on Equation (18).

4. Results and discussion

Table 1 represents the experimental results for the PS nanocomposite samples containing GO or HGO nanoparticles. As it is clear, there has been a significant difference between the thermal conductivity and tensile strength of the samples containing the same amounts of GO and HGO nanoparticles. This is attributed to the advantages of the unique hollow structure of the HGO nanoparticles compared to the layered GO nanoparticles.

Table 1

Results of thermal conduction and tensile tests for the PS nanocomposite samples containing GO or HGO nanoparticles.

Nanoparticle content (Vol. %)	PS containing GO nanoparticles		PS containing HGO nanoparticles	
	$K (W.m^{-1}.K^{-1}) \pm$ STD	E (Gpa) ± STD	$K (W.m^{-1}.K^{-1}) \pm$ STD	E (Gpa) ± STD
0	0.1637±0.054	2.7318±0.06	0.1637±0.054	2.7318±0.06
1	0.6212±0.021	3.0372±0.05	0.7426±0.028	3.1811±0.02
2	0.6936±0.093	3.2454±0.09	0.8061±0.023	3.4569±0.06
3	0.7455±0.076	3.4148±0.03	0.8312±0.031	3.6835±0.04
4	0.7912±0.058	3.5223±0.06	0.8457±0.051	3.8192±0.07

As it is represented by Equations (4) and (17), the analytical model include the thickness of the polymer/particle interphase and the aggregation/agglomeration factor, which can have substantial effects on its final results. We have previously proved that the

thickness of the polymer/particle interphase is dependent on the amount of the nanoparticles and the type of the driving force [11]. Accordingly, it is important to define this parameter in accordance with the results of both thermal conduction and tensile tests for

PS nanocomposites comprising HGO nanoparticles. Tables 2 and 3 represent the results of the analytical model in thermal (Equation (4)) and mechanical (Equation (17)) modes respectively. It should be noted that the tensile modulus of the wall of HGO nanoparticle was considered to be 207 GPa [32].

Table 2

Model results for the thermal conductivity of PS/HGO nanocomposite samples based on Equation (4).

Nanoparticle Content (Vol. %)	Experimental results, K_e (W.K^{-1}.m^{-1})	Model results, K_M (W.K^{-1}.m^{-1})	τ (nm)	μ (%)	K_i (W.K^{-1}.m^{-1})
1	0.7426	0.7484	2.8	0.12	0.132
2	0.8061	0.7901	1.2	0.18	0.144
3	0.8312	0.8255	0.5	0.29	0.155
4	0.8557	0.8327	0.08	0.92	0.158

Table 3

Model results for the tensile modulus of PS/HGO nanocomposite samples based on Equation (17).

Nanoparticle Content (Vol.%)	Experimental results, E_e (GPa)	Model results, E_M (GPa)	τ (nm)	μ (%)	E_i (GPa)
1	3.1811	3.1897	127.6	0.15	2.753
2	3.4569	3.4542	97.2	0.18	2.751
3	3.6835	3.6341	82.5	0.31	2.749
4	3.8192	3.8158	73.1	0.87	2.744

As it is clear, the thickness of the polymer/particle interphase region decreased with increasing the content of the nanoparticle according to both thermal and mechanical model results. Though, the reason for this phenomenon has been comprehensively discussed in references No. [1], [11] and [33]. Also, there was a significant difference between the obtained results for the thickness of the interphase via thermal and mechanical modes of the analytical model, which was attributed to the nature of the system response against the exerted thermal/mechanical deriving force (for more information refer to reference No. [11]).

Based on the results of Table 1, the effects of the HGO nanoparticles on the thermal and mechanical properties of the PS matrix was significantly higher than that of layered GO nanoparticles. On the other hand, according to the results of Tables 2 and 3, the proposed analytical model was completely capable of characterizing the mechanical and thermal properties of PS/HGO nanocomposites. Therefore, it was possible to use the proposed geometrical structure (Figure 1) to simulate the system in order to better understand the differences between the mechanism of the impact of the HGO and layered GO nanoparticles on a polymer matrix.

As it is demonstrated in Figure 4, the heat transfer mechanism in the nanocomposite sample, containing GO and HGO nanoparticles, is substantially different. It should be noted that, according to the simulation results, the heat conduction coefficient in the sample containing GO nanoparticle was 0.6866 (W.K^{-1}.m^{-1}) (the average temperature of the right and the left sides were 36.37 and 109.19 ºC respectively), while that value was 0.8022 (W.K^{-1}.m^{-1}) for the sample containing HGO nanoparticles

(the average temperature of the right and the left sides were 23.86 and 86.19 °C respectively). Those values were very close to the experimentally defined K for the nanocomposite samples containing 2 Vol. % of GO and HGO nanoparticles respectively (Table 1). On the other hand, almost similar results were obtained from the simulation process, analytical modeling, and experimental test (Tables 1 and 2) for the nanocomposite sample containing 2 Vol. % of HGO nanoparticles, which indicated good compatibility between the analytical model and the actual structure of the nanocomposite sample. Also, according to the simulation results, it is clear that the HGO nanoparticles have specific thermal behavior, a uniform temperature at all points of the hollow structure, which we have previously proved, in the case of the cured unsaturated polyester resins containing HGO nanoparticles, they showed their capability as thermal capacitors [16]. Though, this unique capability of these nanoparticles has been introduced as their major advantage compared to GO nanoparticles.
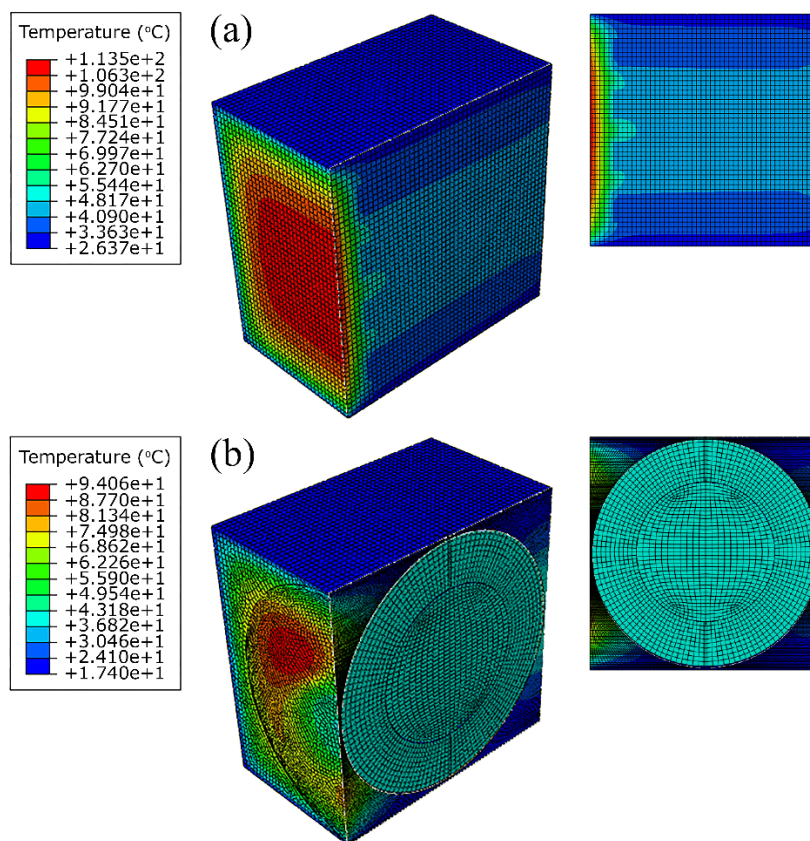

Figure 4. Thermal simulation results for the nanocomposite structures containing (a) GO and (b) HGO nanoparticles.

The results for the mechanical behavior of the simulated nanocomposite samples are represented in Figure 5. The results showed a drastic difference in the mechanical behavior of the samples. As it is clear, the HGO nanoparticles can deal better with the exerted stress since the deformation of the nanocomposite structure containing GO particles is significantly more (Figures 5 (a) and (c)). Furthermore, the results of the stress distribution in the tested structures (Figures 5 (b) and (d)) showed that the HGO

nanoparticles were more involved against the exerted stress, which was also proved via the tensile test results (Table 1). It was also revealed that the hollow structure of HGO

nanoparticles enhanced their mechanical properties as well as their capability to better control environmental conditions.
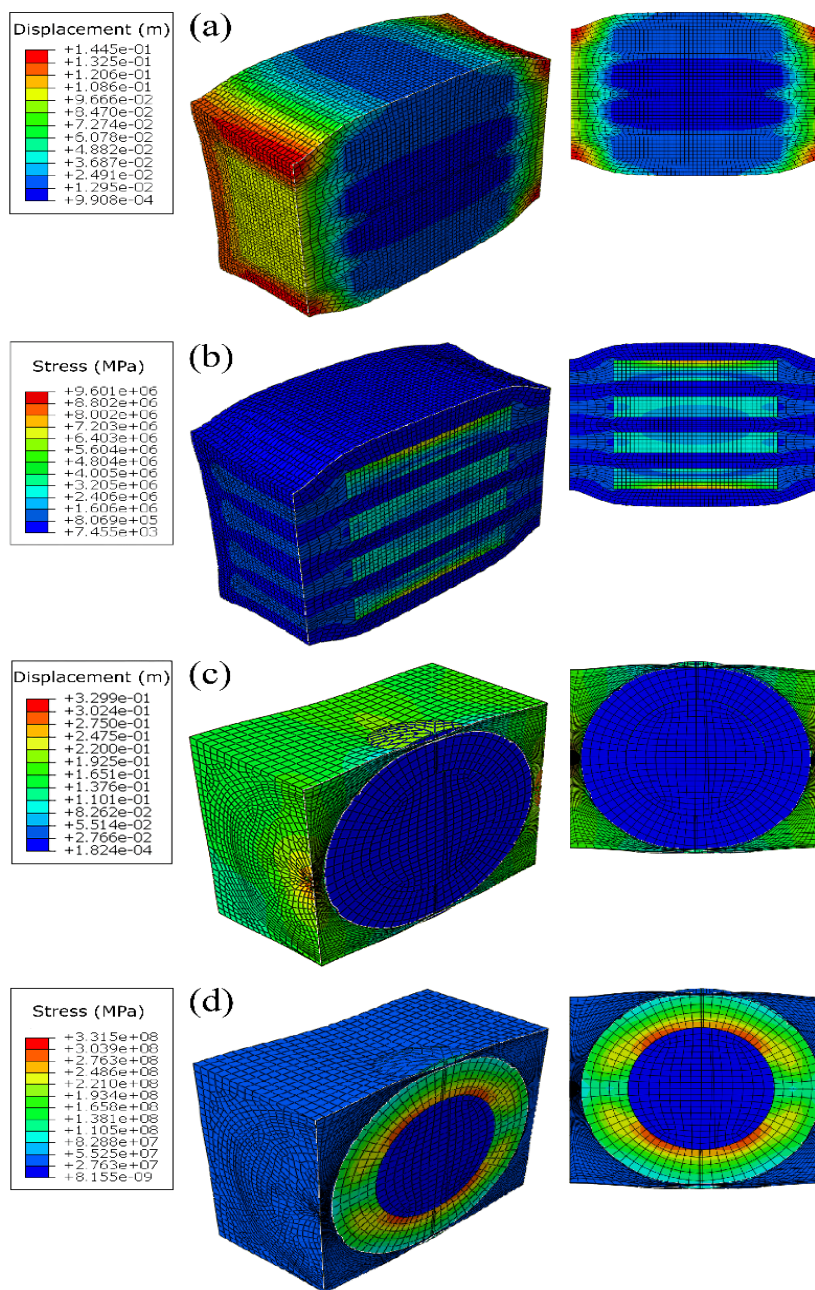

Figure 5. Mechanical simulation results for the nanocomposite structures containing (a)-(b) GO and (c)-(d) HGO nanoparticles.

5. Conclusions

To study the effects of the structure of the nanoparticles on the thermal/mechanical behavior of the nanocomposites, several

samples, containing different amounts of GO and HGO nanoparticles, were prepared for experimental tests. Since some parameters, such as the thickness of the wall, the physical

characteristics of the internal hollow space and the size of the nanoparticles, couldn't be measured experimentally, an analytical model was proposed, based on the EBM and having considered the effects of the characteristics of the polymer/particles and the aggregation/agglomeration factor. The results were used to design the geometrical structures, corresponding to the real system and through a simulation process, using the ABACUS software. Comparing the thermal/mechanical results (the thermal conductivity and tensile strength) of the samples containing the same amounts of GO and HGO nanoparticles, a significant difference was detected, which was ascribed to the unique behavior of the hollow structure of the HGO nanoparticles. Also, the results of the simulation method, analytical modeling, and experimental tests showed that the proposed analytical model was capable of characterizing the mechanical and thermal properties of the nanocomposite samples, through which the positive effect of the HGO nanoparticles on the thermal properties of the nanocomposites was proved. In addition, the HGO nanoparticles performed better in managing the exerted stress than the layered GO nanoparticles, which showed the capability of the HGO nanoparticles in enhancing the mechanical properties.

References

[1] Sharifzadeh, E. and Cheraghi, K., "Temperature-affected mechanical properties of polymer nanocomposites from glassy-state to glass transition temperature", *Mech. Mater.*, **160**, 103990 (2021).

[2] 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).

[3] Sharifzadeh, E., Tohfegar, E. and Safajou Jahankhanemlou, M., "The influences of the nanoparticles related parameters on the tensile strength of polymer nanocomposites", *Iranian Journal of Chemical Engineering (IJChE)*, **17** (1), 65 (2020).

[4] 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).

[5] Sharifzadeh, E. and Amiri, Y., "The effects of the arrangement of Janus nanoparticles on the tensile strength of blend-based polymer nanocomposites", *Polym. Compos.*, **41** (9), 3585 (2020).

[6] 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).

[7] 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).

[8] 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).

[9] 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** (11), 1176 (2019).

[10] Sharifzadeh, E. and Amiri, Y., "The effects of morphological variation and polymer/polymer interface on the tensile modulus of binary polymer blends: A modeling approach", *J. Polym. Eng.*, **41** (2), 109 (2021).

[11] Sharifzadeh, E., "Evaluating the dependency of polymer/particle interphase thickness to the nanoparticles content, aggregation/agglomeration factor and type of the exerted driving force", *Iran. Polym. J.*, **30** (10), 1063 (2021).

[12] Kumar, A., Sharma, K. and Dixit, A. R., "A review on the mechanical properties of polymer composites reinforced by carbon nanotubes and graphene", *Carbon Lett.*, **31** (2), 149 (2021).

[13] Fu, S., Sun, Z., Huang, P., Li, Y. and Hu, N., "Some basic aspects of polymer nanocomposites: A critical review", *Nano Mater. Sci.*, **1** (1), 2 (2019).

[14] Koo, J. H., Fundamentals, properties, and applications of polymer nanocomposites, Cambridge University Press, New York, (2016).

[15] Njuguna, J., Structural nanocomposites: Perspectives for future applications, Springer, Berlin, Heidelberg, (2013).

[16] Pourakbar, E. and Sharifzadeh, E., "Synthesis of Janus/non-Janus hollow graphene oxide micro- and nanoparticles and the effects of their localization on the thermal conductivity of blend-based polymer composites", *J. Mater. Sci.*, **54** (32), 18078 (2021).

[17] Zare, Y., "Study of nanoparticles aggregation/agglomeration in polymer particulate nanocomposites by mechanical properties", *Compos. Part A*

Appl. Sci., **84** (1), 158 (2016).

[18] Santos, R. M., Mould, S. T., Formánek, P., Paiva, M. C. and Covas, J. A., "Effects of particle size and surface chemistry on the dispersion of graphite nanoplates in polypropylene composites", *Polymers*, **10** (2), 222 (2018).

[19] Chanda, S. and Bajwa, D. S., "A review of current physical techniques for dispersion of cellulose nanomaterials in polymer matrices", *Rev. Adv. Mater.*, **60** (1), 325 (2021).

[20] De Gennes, P. G., "Polymers at an interface, 2. Interaction between two plates carrying adsorbed polymer layers", *Macromolecules*, **15** (2), 492 (1982).

[21] Kango, S., Kalia, S., Celli, A., Njuguna, J., Habibi, Y. and Kumar, R., "Surface modification of inorganic nanoparticles for development of organic–inorganic nanocomposites—A review", *Prog. Polym. Sci.*, **38** (8), 1232 (2013).

[22] Tohfegar, E., Moghaddas, J. S., Sharifzadeh, E. and Esmaeilzadeh-Dilmaghani, S., "Synthesis and characterization of waterglass-based silica aerogel under heat treatment for adsorption of nitrate from water: Batch and column studies", *Iranian Journal of Chemical Engineering (IJChE)*, **16** (4), 53 (2019).

[23] Sharifzadeh, E. and Parsnasab, M., "Direct and reverse desymmetrization process in O/W pickering emulsions to produce hollow graphene oxide Janus micro/nano-particles", *Colloids Surf. A Physicochem. Eng.*, **619** (1), 126522 (2021).

[24] Sharifzadeh, E., Salami-Kalajahi, M., Hosseini, M. S. and Razavi Aghjeh, M. K., "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).

[25] Sharifzadeh, E., Salami-Kalajahi, M., Hosseini, M. S. and Razavi Aghjeh, M. K., "A temperature-controlled method to produce Janus nanoparticles using high internal interface systems: Experimental and theoretical approaches", *Colloids Surf. A Physicochem. Eng.*, **506** (1), 56 (2016).

[26] 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).

[27] Zamanian-Fard, A., Sharifzadeh, E. and Rajabi, L., "A spontaneous interfacial process to produce silica Janus nanosheets as perfect emulsifiers in pickering emulsions", *J. Dispersion Sci. Technol.*, **18** (3), 1 (2020).

[28] Perro, A., Meunier, F., Schmitt, V. and Ravaine, S., "Production of large quantities of "Janus" nanoparticles using wax-in-water emulsions", *Colloids Surf. A Physicochem. Eng.*, **332** (1), 57 (2009).

[29] Sharifzadeh, E. and Mohammadi, R., "Temperature-/frequency-dependent complex viscosity and tensile modulus of polymer nanocomposites from the glassy state to the melting point", *Polym. Eng. Sci.*, **61** (10), 2600 (2021).

[30] Pesetskii, S. S. and Bogdanovich, S. P., "Polymer composites and nanocomposites", in Encyclopedia of tribology, Wang, Q. J. and Chung, Y. - W. edition, Springer, Boston, MA., US, p. 2563 (2013).

[31] Shen, J., Wang, M., Li, J., Guo, S., Xu, S., Zhang, Y., Li, T. and Wen, M., "Simulation of mechanical properties of multilayered propylene–ethylene copolymer/ethylene 1-octene copolymer composites by equivalent box model and its experimental verification", *Eur. Polym. J.*, **45** (11), 3269 (2009).

[32] Suk, J. W., Piner, R. D., An, J., and Ruoff, R. S., "Mechanical properties of monolayer graphene oxide", *ACS Nano*, **4** (11), 6557 (2010).

[33] Ader, F. and Sharifzadeh, E., "Rheological and mechanical behavior of blend-based polymer nanocomposites containing Janus and non-Janus silica nanoparticles", *Colloid. Polym. Sci.*, **299** (1), 1843 (2021).