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Упрощенная модель Tandon–Weng для описания модуля упругости при растяжении трехкомпонентных полимерных нанокомпозитов

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Модель Tandon–Weng, основанная на теории Mori–Tanaka для определения модуля упругости при растяжении обычных композитов, в настоящее время применяется для различных полимерных нанокомпозитов. Однако ряд сложных параметров данной модели налагает ограничения при проведении расчетов. В статье предложен упрощенный вариант модели для описания трехкомпонентных полимерных нанокомпозитов, содержащих слоистые и сферические нанонаполнители. Проведено сравнение результатов расчетов на основе разработанной модели с результатами экспериментов, предложено объяснение различия экспериментальных и расчетных данных. Показано, что некоторые параметры модели, например модуль упругости при растяжении наночастиц, не оказывают существенного влияния на модуль упругости при растяжении двух- и трехкомпонентных нанокомпозитов.

Ключевые слова: полимерные нанокомпозиты, трехкомпонентные образцы, теория Mori–Tanaka, модель Tandon–Weng, модуль упругости

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Simplification and development of Tandon–Weng model for tensile modulus of ternary polymer nanocomposites: Comparison of predictions with experimental results

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Tandon–Weng model based on Mori–Tanaka idea for tensile modulus of conventional composites is currently used for various polymer nanocomposites, but some complex terms in this model may limit the calculations. In this article, this model is simplified and developed for ternary polymer nanocomposites containing layered and spherical nanofillers. The calculations of developed model are compared with the experimental results and the trends between experimental data and the predictions are explained. The developed model shows that some parameters such as tensile modulus of nanoparticles cannot significantly affect the tensile modulus of binary and ternary nanocomposites, due to its very high level.

Keywords: polymer nanocomposites, ternary samples, Mori–Tanaka theory, Tandon–Weng model, modulus

1. Introduction

The significant properties of nanostructures relative to conventional materials have attracted a great deal of interest over the last years [1–6]. With the recent progress in nanotechnology, it was reported that the filler size can cause unexpected behavior. However, the material and processing conditions must allow the size of particles to remain or go to the nanoscale. The table depicts the physical and mechanical properties of some nanoparticles used as a nanofiller. The nanoparticles show a very high level of tensile modulus and thus, their low amounts can cause high stiffening effect in the polymer nanocomposites [7]. The excel-

lent reinforcing by nanoparticles is also related to the strong particle–polymer interactions affected by interfacial/interphase characteristics [8]. Therefore, many variables can influence the general properties of polymer nanocomposites and the prediction of the nanocomposite behavior requires to a great knowing of the effective parameters.

The prediction of nanocomposites behavior can help the development and optimization of nanocomposites which will result in the obtaining of desired properties in the final products. Many authors have applied the conventional models suggested for different types of microcomposites for polymer nanocomposites. Some models such as Halpin–

Table

The characteristics of some known nanoparticles

No.	Nanofiller	Density, g·cm ⁻³	Poisson ratio	Tensile modulus, GPa	Shear modulus, GPa
1	Nanoclay	1.8	0.20	180	75.0
2	SiO ₂	2.2	0.17	80	34.2
3	CaCO ₃	2.7	0.27	26	9.9
4	Al ₂ O ₃	3.9	0.26	370	148.0
5	TiO ₂	4.0	0.27	250	98.4

Tsai and Hui–Shia were applied for tensile modulus of polymer nanocomposites [9]. The previous studies can provide valuable information for the effects of some important parameters such as the moduli of polymer matrix and nanofiller, the filler geometry and orientation on the modulus of polymer nanocomposites. Some studies reported the overprediction of the conventional models for polymer/clay nanocomposites [10], while several researches suggested the underprediction of the conventional models, for example the Halpin–Tsai and Guth models for polyamide 66 (PA 66)/CaCO₃ nanocomposite [9]. Moreover, a good consistency between the experimental data and the calculations of the conventional models was reported in Ref. [11]. Conclusively, there is not a definite trend between the experimental data and the model predictions for polymer nanocomposites and the estimation of the tensile modulus by conventional models is challenging.

Many parameters control the tensile modulus of nanocomposites such as content, dimensions, moduli and dispersion/agglomeration of nanoparticles in addition to the characteristics of interface/interphase regions between polymer and nanofiller [12, 13]. However, the correct measurements of several parameters such as aspect ratio, orientation and dispersion/agglomeration of nanoparticles along with the interfacial/interphase properties are difficult or impossible, due to the manipulating of nanoscale and atomic interactions at interface/interphase areas.

In our previous work, Tandon–Weng model based on Mori–Tanaka theory was simplified for polymer nanocomposites containing spherical nanoparticles [14]. The simplified model was developed assuming interphase regions between polymer matrix and nanoparticles. In this paper, the simplified Tandon–Weng model is developed for ternary polymer nanocomposites containing layered and spherical nanofillers. The developed model is applied to calculate the moduli of several binary and ternary samples and the trends between experimental and theoretical results are described and justified.

2. Theoretical views

2.1. Mori–Tanaka model

The longitudinal and transverse elastic moduli are generally expressed by Tandon–Weng model based on Mori–

Tanaka theory [15, 16] as

$$\frac{E_{11}}{E_m} = \frac{1}{1 + \varphi_f (A_1 + 2\nu_m A_2)/A_6}, \quad (1)$$

$$\frac{E_{22}}{E_m} = \frac{1}{1 + \varphi_f [-2\nu_m A_3 + (1 - \nu_m)A_4 + (1 + \nu_m)A_5 A_6]/(2A_6)}, \quad (2)$$

where E_m and ν_m are the tensile modulus and Poisson ratio of matrix, respectively, φ_f is also the volume fraction of nanofiller. The parameters $A_1, A_2, \dots, A_6$ are functions of the Eshelby's tensor and the properties of the filler and matrix as

$$A_1 = D_1(B_4 + B_5) - 2B_2, \quad (3)$$

$$A_2 = (1 + D_1)B_2 - (B_4 + B_5), \quad (4)$$

$$A_3 = B_1 - D_1 B_3, \quad (5)$$

$$A_4 = (1 + D_1)B_1 - 2B_3, \quad (6)$$

$$A_5 = (1 - D_1)/(B_4 - B_5), \quad (7)$$

$$A_6 = 2B_2 B_3 - B_1(B_4 + B_5), \quad (8)$$

where D_1, D_2 and D_3 are functions of the Lamé constants of the matrix and particles as

$$D_1 = 1 + 2(\mu_f - \mu_m)/(\lambda_f - \lambda_m), \quad (9)$$

$$D_2 = (\lambda_m + 2\mu_m)/(\lambda_f - \lambda_m), \quad (10)$$

$$D_3 = \lambda_m/(\lambda_f - \lambda_m), \quad (11)$$

$$\lambda = \frac{Ev}{(1 + \nu)(1 - 2\nu)}, \quad (12)$$

$$\mu = \frac{E}{2(1 + \nu)}, \quad (13)$$

where λ and μ are the Lamé's first and second constants, respectively. E and ν show the tensile modulus and Poisson ratio, respectively and m and f subscripts indicate the matrix and filler phases, respectively. The B_i parameters are also defined as

$$B_1 = \varphi_f D_1 + D_2 + (1 - \varphi_f)(D_1 S_{1111} + 2S_{2211}), \quad (14)$$

$$B_2 = \varphi_f + D_3 + (1 - \varphi_f)(D_1 S_{1122} + S_{2222} + S_{2233}), \quad (15)$$

$$B_3 = \varphi_f + D_3 + (1 - \varphi_f)[S_{1111} + (1 + D_1)S_{2211}], \quad (16)$$

$$B_4 = \varphi_f D_1 + D_2 + (1 - \varphi_f) \times \\ \times [S_{1122} + D_1 S_{2222} + S_{2233}], \quad (17)$$

$B_5 = \varphi_f + D_3 + (1 - \varphi_f)(S_{1122} + S_{2222} + D_1 S_{2233})$, (18)
where parameters S_{ijkl} depend to v_m and aspect ratio of particles α for layered filler as

$$S_{1111} = \frac{1}{2(1 - v_m)} \left[1 - 2v_m + \right. \\ \left. + \frac{3\alpha^2 - 1}{\alpha^2 - 1} \left(1 - 2v_m + \frac{3\alpha^2}{\alpha^2 - 1} \right) g \right], \quad (19)$$

$$S_{2222} = \frac{3}{8(1 - v_m)} \frac{\alpha^2}{\alpha^2 - 1} + \\ + \frac{1}{4(1 - v_m)} \left[1 - 2v_m - \frac{9}{4(\alpha^2 - 1)} \right] g, \quad (20)$$

$$S_{2233} = \frac{1}{4(1 - v_m)} \left\{ \frac{\alpha^2}{2(\alpha^2 - 1)} - \right. \\ \left. - \left[1 - 2v_m + \frac{3}{4(\alpha^2 - 1)} \right] g \right\}, \quad (21)$$

$$S_{2211} = -\frac{1}{2(1 - v_m)} \frac{\alpha^2}{(\alpha^2 - 1)} + \\ + \frac{1}{4(1 - v_m)} \left[\frac{3\alpha^2}{\alpha^2 - 1} - 1 + 2v_m \right] g, \quad (22)$$

$$S_{1122} = -\frac{1}{2(1 - v_m)} \left(1 - 2v_m + \frac{1}{\alpha^2 - 1} \right) + \\ + \frac{1}{2(1 - v_m)} \left[1 - 2v_m + \frac{3}{2(\alpha^2 - 1)} \right] g, \quad (23)$$

$$S_{2323} = \frac{1}{4(1 - v_m)} \left\{ \frac{\alpha^2}{2(\alpha^2 - 1)} + \right. \\ \left. + \left[1 - 2v_m - \frac{3}{4(\alpha^2 - 1)} \right] g \right\}, \quad (24)$$

$$S_{1212} = \frac{1}{4(1 - v_m)} \left\{ 1 - 2v_m - \frac{\alpha^2 + 1}{\alpha^2 - 1} - \right. \\ \left. - 0.5 \left[1 - 2v_m - \frac{3(\alpha^2 + 1)}{\alpha^2 - 1} \right] g \right\}, \quad (25)$$

$$g = \frac{\alpha}{(1 - \alpha^2)^{3/2}} [\cos^{-1} \alpha - \alpha(1 - \alpha^2)^{1/2}], \quad (26)$$

α for disc-like platelets is defined as t/d , where t and d are the thickness and diameter of the platelets.

The parameters S_{ijkl} for spherical particles can be expressed by

$$S_{1111} = S_{2222} = S_{3333} = \frac{7 - 5v_m}{15(1 - v_m)}, \quad (27)$$

$$S_{1122} = S_{2233} = S_{2211} = \frac{5v_m - 1}{15(1 - v_m)}. \quad (28)$$

For a ternary sample containing two types of nanoparticles, the longitudinal and transverse moduli are expressed by Mori–Tanaka model as

$$\frac{E_{11}}{E_m} = [1 + \varphi_{fl}(A_{1l} + 2v_m A_{2l})/A_{6l} + \\ + \varphi_{fs}(A_{1s} + 2v_m A_{2s})/A_{6s}]^{-1}, \quad (29)$$

$$\frac{E_{22}}{E_m} = (1 + \varphi_{fl}[-2v_m A_{3l} + (1 - v_m)A_{4l} + \\ + (1 + v_m)A_{5l}A_{6l}]/(2A_{6l}) + \dots)^{-1} + \\ + \varphi_{fs}[-2v_m A_{3s} + (1 - v_m)A_{4s} + \\ + (1 + v_m)A_{5s}A_{6s}]/(2A_{6s}), \quad (30)$$

where l and s subscripts indicate the layered and spherical nanoparticles, respectively. The tensile modulus of binary and ternary samples can be calculated by the suggested model for 3D randomly dispersed particles [11] as

$$E_r = 0.49 \frac{E_{11}}{E_m} + 0.51 \frac{E_{22}}{E_m}, \quad (31)$$

where E_r is defined as E_c/E_m , E_c is the tensile modulus of nanocomposite. It should be noted that the longitudinal and transverse moduli for binary nanocomposites reinforced with spherical nanoparticles are equal.

2.2. Simplification of the model

The parameters can be simplified for polymer/clay binary nanocomposites assuming $v_f = 0.2$, $v_m \approx 0.4$, $E_m \approx 2$ GPa, $E_f \approx 180$ GPa and $\alpha < 0.01$ as

$$g \approx 0, \quad (32)$$

$$S_{1111} \approx 1, \quad (33)$$

$$S_{2222} = S_{2233} = S_{2211} = S_{2323} \approx 0, \quad (34)$$

$$S_{1122} \approx \frac{v_m}{1 - v_m}, \quad (35)$$

$$S_{1212} \approx 0.5, \quad (36)$$

$$D_1 \approx 4.2, \quad (37)$$

$$D_2 = D_3 \approx 0.1, \quad (38)$$

$$B_1 = 4.25, \quad (39)$$

$$B_2 = \varphi_f + \frac{4.2v_m}{1 - v_m}, \quad (40)$$

$$B_3 = 1.1, \quad (41)$$

$$B_4 = 4.2\varphi_f + 0.15 + \frac{v_m}{1 - v_m}, \quad (42)$$

$$B_5 = \varphi_f + 0.1 + \frac{v_m}{1 - v_m}, \quad (43)$$

$$A_1 = 25\varphi_f + 1, \quad (44)$$

$$A_2 = \frac{20v_m}{1 - v_m} - 0.25, \quad (45)$$

$$A_3 = -0.2, \quad (46)$$

$$A_4 = 20, \quad (47)$$

$$A_5 = \frac{-1}{\phi_f + 0.02}, \quad (48)$$

$$A_6 = -25\phi_f + \frac{0.7v_m}{1-v_m} - 1.1. \quad (49)$$

For spherical nanoparticles, the simplified parameters and their details were reported in our previous work [14].

3. Experimental

Several ternary samples of polypropylene (PP)/nano-clay/ CaCO_3 at different weight percentages of both nanofillers were prepared and tested. PP homopolymer (ZH500, MFI = 10 g/10 min, 230°C, 2.16 kg) was supplied from Navid Zar Shimi Company, Iran. A montmorillonite clay modified with a quaternary ammonium salt based on hydrogenated tallow (Cloisite20A type) was provided from Southern Clay Products. The maleic anhydride grafted PP (PPgMA) compatibilizer was supplied as PB3150 (MFI = 20 g/10 min, 230°C, 2.16 kg) with 0.5 wt % of maleic anhydride. The precipitated CaCO_3 (Socal312, 70 nm, coated with stearic acid) was provided from Solvay.

The melt mixing of samples was performed by a co-rotating twin screw extruder, Brabender TSE 20/40D ($D = 20$ mm, $L/D = 40$). The screw speed and the feeding rate were kept at 250 rpm and 3 kg/h, respectively. The temperature profile was fixed from hopper to die at 210 to

230°C. The injection molding was performed using a Mono-Mat 80 injection molding machine at melt and mold temperatures of 245 and 80°C, respectively. The tensile test was performed using Z050, Zwick according to ASTM D638 at crosshead speed of 50 mm/min.

4. Results and discussion

The suggested equations are applied to calculate the tensile modulus in some reported samples from the literature and the own prepared ternary samples. Additionally, the calculations are compared with the experimental data.

Figure 1 exhibits the predictions of the simplified model for several binary nanocomposites containing spherical nanoparticles reported in the literature. It is revealed that the simplified model underpredicts the tensile modulus of the reported samples. This trend is also found in other samples such as PP/ CaCO_3 [20] and linear low density polyethylene (LLDPE)/ SiO_2 [21]. As a result, it can be concluded that the Mori–Tanaka model generally underpredicts the tensile modulus of the spherical-nanoparticles reinforced nanocomposites, i.e. the experimental data are higher than the theoretical predictions. This finding is well agreed with the observations of Sisakht et al. [9], where the conventional models such as Guth, Halpin–Tsai, Hashin–Shtrikman and inverse rule of mixtures underpredicted the tensile modulus of PA66/ CaCO_3 nanocomposite. The small nanoparticle size, which introduces a greater surface area, can provide more filler–filler and polymer–filler interaction/adhesion at atomic scale. As a result, the nanoparticles can cause

Fig. 1. The predictions of the simplified model for polyamide 66 (PA66)/ SiO_2 [17] (a), poly(vinyl chloride) (PVC)/ CaCO_3 [18] (b), high impact polystyrene (HIPS)/ TiO_2 [19] (c) and PA 66/ CaCO_3 [9] samples (d)

more effective reinforcement than that of the theoretical models express. In other words, the conventional models cannot regard the reinforcing effects of nanoparticles in polymer nanocomposites, which are provided by the interfacial interaction/adhesion, i.e. interphase formation. Many articles in the literature indicated to the mentioned effect of nanoparticles in polymer matrixes which is caused by the high surface area of the nanoparticles and the nano-scale interactions [22, 23]. For example, Ji et al. [24] introduced the thickness and tensile modulus of the interphase in two-phase Takayanagi model and developed a suitable three-phase model for the tensile modulus of nanocomposites. The developed models indicated the important role of the interphase in the mechanical behavior of nanocomposites.

Figure 2 displays the experimental data for the prepared ternary samples in this study and the reported results in the literature as well as the calculations of the developed model. The predictions are higher than the experimental results at all nanofiller weight percentages. It may be stated that the simplified Mori–Tanaka model overpredicts the tensile modulus of ternary polymer nanocomposites containing layered and spherical nanoparticles. Other conventional models such as Halpin–Tsai and its derivations for polymer/clay nanocomposites have described this trend (overprediction) [10]. As a result, it is understood that the clay platelets play the main role in the ternary samples. This assumption is logical, because the clay platelets induce higher surface area and nucleation sites and significant re-

inforcing effect compared to CaCO_3 nanoparticles [25]. Basically, this Mori–Tanaka model assumes that the nanoparticles are perfectly aligned, asymmetric and uniform in shape and size [16]. Moreover, the behavior of matrix and nanofiller in nanocomposite is identically considered to those of the neat materials. No particle–particle and strong polymer–particle interactions are taken into account in this model. However, some undesirable phenomena such as the weak dispersion of nanoparticles or poor exfoliation of clay platelets, the various values of length and thickness of platelets, the aggregation/agglomeration of nanoparticles especially at high nanofiller content in ternary samples, the poor interfacial adhesion at the polymer–filler interface and the particle–particle interaction are shown in polymer nanocomposites in practice [26, 27]. One or more of the above phenomena is enough to decrease the modulus of nanocomposites, which results in the low modulus compared to the prediction of the simplified Mori–Tanaka model.

On the other hand, the conventional models such as Mori–Tanaka do not assume the roles and influences of polymer–particle and particle–particle interfacial interactions, interphase between polymer and nanofiller and the dispersion/aggregation level of nanoparticles in polymer matrix, while it was reported that these factors considerably affect the tensile modulus of polymer nanocomposites [28, 29]. It was indicated that the interphase occupies a high volume fraction in polymer nanocomposites and disregarding it causes the incorrect estimation of the tensile

Fig. 2. The predictions of the developed model for PP/nanoclay/ CaCO_3 ternary nanocomposites: own samples at 2 wt % nanoclay (a), own samples at 4 wt % nanoclay (b), own samples at 6 wt % nanoclay (c) and the reported results [20] (d)

modulus [30, 31]. Furthermore, the nanoparticles generally tend to aggregation/agglomeration in the fabrication process of samples affecting the properties of nanocomposites [32, 33]. It is understood that the conventional models cannot properly predict the mechanical properties of the nanocomposites without supposing the influences of these factors.

The conventional models such as Mori–Tanaka assumed the influences of α , v_m , E_f and v_f on the final tensile modulus. However, it was shown that α cannot meaningfully change the tensile modulus and its effect is removed (g was assumed as 0), because α gets a very low value for nanoplatelets (<0.01). The limited and low values of v_m and v_f parameters (below 0.5) cannot significantly vary the calculations of the conventional models, because the high level of E_f removes their influences in polymer nanocomposites. However, the simplicity of the conventional models leads to their wide application for different polymer nanocomposites at the first step of behavior prediction or for an initial estimation or to answer this important question that whether these models are appropriate for polymer nanocomposites or not.

5. Conclusions

Tandon–Weng model based on Mori–Tanaka theory for tensile modulus of composites was simplified and developed for ternary polymer nanocomposites. The calculations of the developed model were also likened with the experimental results of many samples. Although original model assumed that many characteristics of the polymer matrix and filler such as Poisson's ratio, moduli, concentration and aspect ratio govern the tensile modulus, it was found that the aspect ratio of nanofiller and the tensile modulus of nanoparticles cannot change the tensile modulus of binary and ternary nanocomposites. The developed simplified model displayed that the tensile modulus only depends to Poisson's ratio of the matrix and nanofiller concentration. It was found that the simplified model underpredicts the modulus of binary nanocomposites containing spherical particles. This occurrence was attributed to the greater reinforcing effect of nanoparticles, which is obtained by strong interfacial interactions between polymer matrix and nanoparticles. The developed model for ternary samples also revealed the overprediction of the tensile modulus compared to experimental results. It was explained that some undesirable phenomena such as poor dispersion of nanoparticles, aggregation/agglomeration of nanoparticles especially at high nanofiller content, poor interfacial adhesion at polymer–filler interface and particle–particle interactions may decrease the tensile modulus of ternary samples in practice.

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