Effects of Particle Agglomeration and Interphase on Nonacomposites

Jing Pan[1,a], Li-chun Bian[1,b] and Ming Gao[1,c]
[1]*Key Laboratory of Mechanical Reliability for Heavy Equipments and Large Structures of Hebei Province*
Yanshan University, Qinhuangdao 066004, PR China

Keywords: Particle, agglomeration, interphase, Composite.

Abstract: In this paper, a simple approach is described to investigate the effects of particle content, presence of interphase and agglomeration on the effective modulus of nanocomposites. A new micromechanical agglomeration model and the Mori-Tanaka method are applied to account for these effects. In the process of derivation, the composite is divided into two parts and the particles encapsulated by an interphaseare regarded as a system. The main effects of nanoparticle radius and interphase thickness, as well as interphase properties, on elastic modulus of nanocomposites are also discussed. The findings show that the nanoparticle agglomeration significantly reduces the effective elastic modulus of composites.

1 INTRODUCTION

Particle-reinforced composites have been received much attention due to their advantages over conventional materials (Cheng et al., 2014; Odegard et al., 2004; Pontefisso et al., 2013). The exceptional properties of nanocompositesare related to small particle size, which results in great interfacialproperties between nanofiller and polymer matrix.The properties of interphase in polymer composites are often different from those of bulk polymer matrix, which may include chemical, physical, microstructural, and mechanical properties. The nature of interphase is critical to the overall properties and performance of polymer materials, in particular in nanofiller reinforced composites (Xu et al., 2016).The small size and high surface per unit volume of nanoparticles leads to strong attractive interaction between particles. So the nanoparticles can be easily agglomerated when added to matrix (Zare et al., 2017; Zare, 2016).

In recent years, several theoretical investigations on particles agglomeration and interphaseproperties have presented much information to attain desirable properties in nanocomposites.Effect of inter-particle interactions on the effective dielectricconstant was calculated as a function of filler volume fraction,packing density of particles inside agglomerates and agglomerate size (Golbang et al., 2017).Afinite element modelling is utilized to investigate the effect of nanoparticle agglomeration on the glass transition temperature of polymer nanocomposites (Qiao et al., 2011). The Halpin-Tsai micromechanical model is modified to account for theeffect of interphase and filler agglomerates and the model predictions for the effective modulus of the composites arecompared to the experimental data. The interphase width and modulus and theagglomerate size were determined based onatomic force microscopy (Karevan et al., 2010). A straightforward analytical approach is presented to estimate effective elastic properties of composites comprising particles encapsulated by an interphase of finite thickness and distinct elastic properties. This explicit solution can treat nanocomposites that comprise either physically isolated nanoparticles or agglomerates of such nanoparticles (Deng and Van Vliet, 2011).

2 AGGLOMERATION MODEL

Dispersion and agglomeration control the macroscopic properties of nanocomposites, thus, quantitative characterization of particle dispersion and agglomeration is crucial. According to the theoretical and experimental research, the particles are easy to agglomerate in matrix. In order to study the effect of particles agglomeration, we proposed an agglomeration model as shown in Figure 1. L_m, L_I and L_p are the stiffness tensor of matrix, interphase and particle, respectively. The stiffness tensor of composites and agglomerated particles are denoted by L and L_a . In the present model,the particles encapsulated by an interphaseare considered as a system. The entire composite is divided into two parts: one part is the particle agglomeration regions, the other part is randomly dispersed particles in matrix.

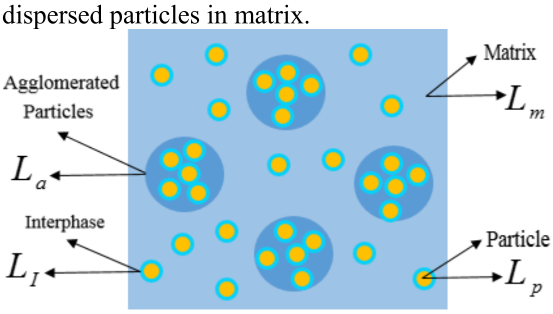

Figure 1: The agglomeration model of nanoparticles.

2.1 Theory Formula

According to the above analysis, the volume fractions of matrix, particle and interphase are defined by f_m , f_p and f_I . So, we get:

$$f_p + f_I + f_m = 1 \tag{1}$$

The volume fraction of interphase is related to that of particle, so, we have:

$$f_I = f_p\left[\left(1+t/r\right)^3 - 1\right] \tag{2}$$

Based on the present model, we introduce an agglomeration parameter ξ to describe the agglomerated degree of particles.

$$\xi = V_a / V \tag{3}$$

here V_a and V are the total volume of particles agglomeration regions and representative volume element, respectively. The volume ratio of particles that are dispersed in agglomerated regions and the total volume of the particles is denoted by λ .

$$\lambda = V_a^p / V_p \tag{4}$$

Equations (1)-(4) correspond to Fig. 1 and they will be applied in the following analysis.

2.2 The Effective Modulus of Composites

The effective modulus of composites based on Mori-Tanaka method is expressed as follow:

$$K = K_b\left[1 + \frac{\xi(K_a - K_b)}{K_b + \alpha(1-\xi)(K_a - K_b)}\right] \tag{5}$$

$$G = G_b\left[1 + \frac{\xi(G_a - G_b)}{G_b + \beta(1-\xi)(G_a - G_b)}\right] \tag{6}$$

Here, K and G are bulk modulus and shear modulus of composites. α and β are constants, and related to the Poisson's ratio of the materials.

In the same way, the bulk modulus K_a and shear modulus G_a of agglomeration regions can be derived.

$$K_a = K_m\left\{1 + \frac{c_1(K_{Ipa} - K_m)}{K_m + \alpha_m c_2(K_{Ipa} - K_m)}\right\} \tag{7}$$

$$G_a = G_m\left\{1 + \frac{c_1(G_{Ipa} - G_m)}{G_m + \beta_m c_2(G_{Ipa} - G_m)}\right\} \tag{8}$$

here, $c_1 = (f_p + f_I)\lambda$

$$c_2 = \xi - \left(f_p + f_I\right)\lambda$$

The bulk modulus K_b and shear modulus G_b of random dispersed particles reinforced composite are as follow:

$$K_b = K_m\left\{1 + \frac{c_3(K_{Ipb} - K_m)}{K_m + \alpha_m c_4(K_{Ipb} - K_m)}\right\} \tag{9}$$

$$G_b = G_m\left\{1 + \frac{c_3(G_{Ipb} - G_m)}{G_m + \beta_m c_4(G_{Ipb} - G_m)}\right\} \tag{10}$$

here, $c_3 = f_p(1-\lambda) + f_I(1-\lambda)$

$$c_4 = (1-\xi) - \left[f_p(1-\lambda) + f_I(1-\lambda)\right]$$

The bulk modulus K_{Ipa} and shear modulus G_{Ipa} of particle-interphase system in agglomerated regions can be expressed.

$$K_{Ipa} = K_I \left\{ 1 + \frac{c_5(K_p - K_I)}{K_I + \alpha_I c_6 K_p - K_I)} \right\} \quad (11)$$

$$G_{Ipa} = G_I \left\{ 1 + \frac{c_5(G_p - G_I)}{G_I + \beta_I c_6 (G_p - G_I)} \right\} \quad (12)$$

here, $c_5 = f_p \lambda$, $c_6 = f_I \lambda$.

Similarly, the bulk modulus K_{Ipb} and shear modulus G_{Ipb} of particle-interphase system randomly dispersed in the original matrix.

$$K_{Ipb} = K_I \left\{ 1 + \frac{c_7(K_p - K_I)}{K_I + \alpha_I c_8 (K_p - K_I)} \right\} \quad (13)$$

$$G_{Ipb} = G_I \left\{ 1 + \frac{c_7(G_p - G_I)}{G_I + \beta_I c_8 (G_p - G_I)} \right\} \quad (14)$$

here, $c_7 = f_p(1-\lambda)$, $c_8 = f_I(1-\lambda)$

The effective elastic modulus of composite consists of two parts have obtained. In the process of analysis, the particles agglomerated state and radius, as well as the interphase thickness and properties are also considered.

3 RESULTS AND DISCUSSION

In this part, the effect of particles agglomeration on the effective modulus of composites is predicted. Moreover, the influences of particle radius and interphase thickness are discussed. The materials properties are from Cheng's work (Cheng et al., 2014).

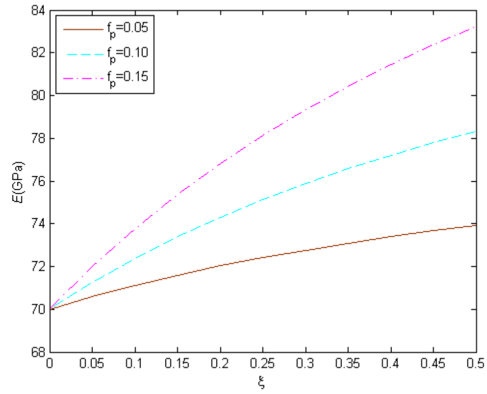

Figure 2: The variation of effective modulus of composites with agglomeration parameter ξ.

Figure 2 presents the variation of effective modulus of composites with agglomeration parameter ξ. It can be seen that the effective modulus of composites monotonically increases with the increase of agglomeration parameter ξ. The reason could be that the particles agglomeration more loosely with increasing parameter ξ. With increasing the volume fractions of particles, the effective modulus of composites increases. So, the increase of particles volume fraction apply to a reinforcing effect for the composites.

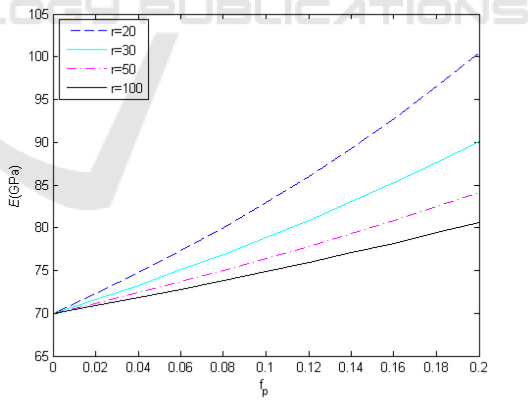

Figure 3: The variation of elastic modulus of composites with particles radius at different particles volume fraction.

The effect of particle radius on the elastic modulus of composites is depicted in Figure 3. The elastic modulus of composites decreases with the increase of particles radius as shown in Figure 3. Therefore, the increase of particle radius reduces the effective elastic modulus of composites. But, the increase of particles volume fraction increases the effective elastic modulus of composites.

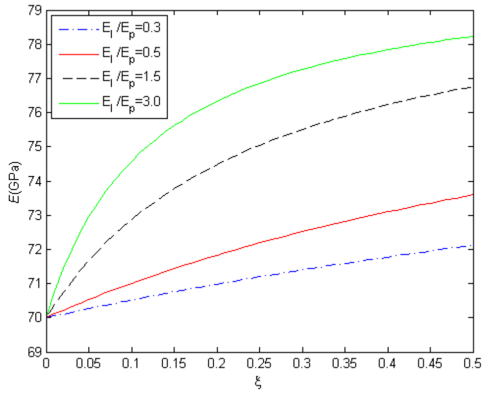

Figure 4: The effect of interphase properties on the elastic modulus of composites.

Figure 4 depicts results of elastic modulus of composites versus relative interphase stiffness E_I / E_p based on the present approach. It is found from Figure 4 that the effective modulus increases with the increase of both the relativeinterphase stiffness E_I / E_p and the agglomeration parameter ξ. That is, for a given particle stiffness $E_p = 427\text{GPa}$, an increase in interphase stiffness increases the elastic modulus of composites.

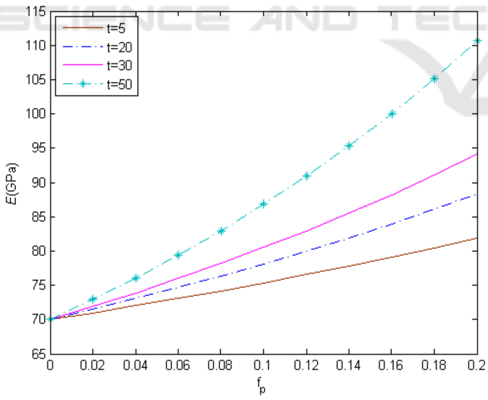

Figure 5: The effect of interphase thickness on the effective elastic modulus of composites.

The effect of interphase thickness on the effective elastic modulus of composites is shown in Figure 5. The effective elastic modulus of composites increases with the increase of both interphase thickness and particles volume fraction. The increase of interphase thickness and particles volume fractions play an important role in improving the effective properties of composites.

4 CONCLUSIONS

In this article, a new particle agglomeration model is proposed to study the influences of particle radius and interphase thickness on the effective modulus of composites. In the process of derivation, an agglomeration parameter is introduced to denote the agglomerated degree of particles. The calculated results show that the agglomerated particles and interphase properties have a significant effect on the composites. The nonuniform dispersion of particles in the matrix reduces the overall stiffness of composites.

ACKNOWLEDGEMENTS

This research was supported by the Science Research Foundation of Hebei Advanced Institutes (ZD2017075) and Graduate Innovation Research Assistant Support Project of Yanshan University (CXZS201708).

REFERENCES

1. Cheng Y, Bian L, Wang Y, et al., 2014. Influences of reinforcing particle and interface bonding strength on material properties of Mg/nano-particle composites. *International Journal of Solids & Structures*, 51(18):3168-3176.
2. Odegard G M, Clancy T C, Gates T S., 2005.Modeling of the mechanical properties of nanoparticle/polymer composites. *Polymer*, 46(2):553-562.
3. Pontefisso A, Zappalorto M, Quaresimin M., 2013. Influence of interphase and filler distribution on the elastic properties of nanoparticle filled polymers. *Mechanics Research Communications*, 52(4):92-94.
4. Xu W, Zeng Q H, Yu A B, et al., 2017.Determination of Interphase Thickness and Mechanical Properties of Effective Nanofillers in Polymer Nanocomposites by Molecular Dynamic Simulation. *Materials Science Forum*, 654-656:1654-1657.
5. Zare Y, Rhee K Y, Hui D., 2017. Influences of nanoparticles aggregation/agglomeration on the interfacial/interphase and tensile properties of nanocomposites. *Composites Part B Engineering*, 122:41-46.
6. Zare Y., 2016. Study of nanoparticles aggregation/agglomeration in polymer particulate nanocomposites by mechanical properties. Composites. *Part A Applied Science & Manufacturing*, 84:158-164.
7. Golbang A, Famili M H N, Shirvan M MM., 2017. A method for quantitative characterization of

agglomeration degree in nanocomposites. *Composites Science & Technology*, 145:181-186.

8. Qiao R, Deng H, Putz K W, et al., 2011. Effect of particle agglomeration and interphase on the glass transition temperature of polymer nanocomposites. *Journal of Polymer Science Part B Polymer Physics*, 49(10):740-748.
9. Karevan M, Pucha R V, Bhuiyan M A, et al., 2010. Effect of Interphase Modulus and Nanofiller Agglomeration on the Tensile Modulus of Graphite Nanoplatelets and Carbon Nanotube Reinforced Polypropylene Nanocomposites. *Carbon Lett*, 11(4):325-331.
10. Deng F, Van Vliet K J., 2011.Prediction of elastic properties for polymer-particle nanocomposites exhibiting an interphase. *Nanotechnology*, 22(16):165703.