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Influence of adhesive energy on debonding in polymeric composites containing randomly located nanoparticles

B. J. Yang[1)] and *H. K. Lee[2)]

[1), 2)] Department of Civil and Environmental Engineering,
Korea Advanced Institute of Science and Technology,
291 Daehak-ro, Yuseong-gu, Daejeon 305-701, Republic of Korea
[2)] leeh@kaist.ac.kr

ABSTRACT

Since the classical damage model neglects the particle size and its interface properties, it is not suitable for the modeling of nanocomposites which have relatively large interfacial area. This paper summarizes a portion of work done by the authors (Yang et al., 2013a) conducted to carry out a parametric study of adhesive energy on the behavior of nanoparticle-reinforced polymeric composites. A micromechanics-based constitutive model (Ju and Lee, 2000; Yang et al., 2013b) for nanoparticulate composites is utilized and influences of adhesive energy at interface region on the overall behavior of nanocomposites are discussed to elucidate the potential of the proposed approach (Yang et al., 2013a).

1. INTRODUCTION

Nanoparticulate composites exhibit an extraordinary performance due to the nanoscale fillers, which generally have dimension range in 0.1 to 100 nm (Kim et al., 2011). It is empirically demonstrated that the addition of rigid nanoparticles to polymer matrix increases the strength of the materials (Fu et al., 2008; Zhang et al., 2008), and thus the nanoparticle-reinforced polymeric composites have a high potential to play an important role in the future (Yang et al., 2013a). A rising issue concerning such nanocomposites is the interface surface between polymer and nanoparticles since an interface surface area is extremely increased compared to microscale materials (Yao et al., 2006). The variations in the interface properties must therefore be considered for an accurate prediction of the overall behavior of nanocomposites.

This paper summarizes a recent work done by the authors (Yang et al., 2013a), and the effects of adhesive energy on the behavior of nanocomposites are discussed. Since the classical damage model neglects the interfacial properties of composite materials, a micromechanical damage model including interface and size effects is considered in the present study (Yang et al., 2013a). Based on the model, the influences of the adhesive energy between nanoparticle and matrix are examined via numerical simulations.

2. Micromechanical damage model for nanoparticulate composites

The Eshelby tensor for a nano-inhomogeneity proposed by Duan et al., (2005) is incorporated into a micromechanics-based framework to consider the interface effect of the nanocomposites (Yang et al., 2013a). We consider that the nanocomposites is comprised of polymer matrix (phase 0) and uniformly dispersed nanoparticles (phase 1). Following the method proposed by Ju and Chen (1994) and Kim et al., (2011), the effective elastic constitutive equation of the nanocomposites can be written as (Ju and Chen, 1994; Yang et al., 2013b)

$$\mathbf{C}_* = \mathbf{C_0}\{\mathbf{I} + \mathbf{B}\,?(\mathbf{I} \quad \mathbf{S}\;\mathbf{B})^{-1}\} \tag{1}$$

with

$$\mathbf{B} = f_1(\mathbf{S} + (\mathbf{C}_1 - \mathbf{C}_0)^{-1}\mathbf{C}_0)^{-1} \tag{2}$$

where $\mathbf{C}_r$ (r=0, 1) denotes stiffness tensor of matrix and nanoparticles, $\mathbf{I}$ is a fourth-rank tensor, and ϕ_1 signifies volume fraction of nanoparticles, respectively. The ensemble volume-averaged Eshelby tensor $\mathbf{S}$ for a spherical nanoscale inclusion with interface effect (Duan et al., 2005) is given in Kim et al., (2011). The Weibull's probabilistic model (Weibull, 1965) has been adopted to describe the damage mechanism of composite materials (e.g., Ju and Lee, 2000; Pyo and Lee, 2010).Furthermore, the critical debonding stress is considered in this study for illustration of interfacial damage response (Fu et al., 2008; Zhang et al., 2008). Details of the damage modeling and the critical debonding stress can be found in Yang et al. (2013a).

3. NUMERICAL SIMULATIONS

Numerical simulations based on the aforementioned micromechanical model are conducted to investigate the effect of the adhesive energy on the behavior of SiO_2 nanoparticle reinforced polyimide matrix (Odegard et al., 2005). The overall relations of critical debonding stress versus radius of nanoparticles at increasing interfacial adhesive energy are illustrated in Figure 1, indicating that the nanoparticle debonding becomes less pronounced as the particle size R decreases (Yang et al., 2013a). Details of the numerical simulations will be presented.

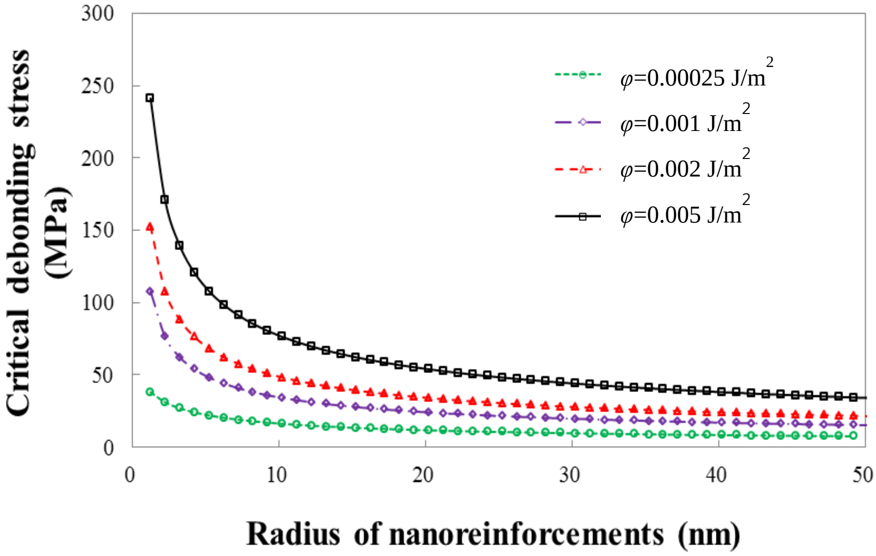

Figure 1. Effects of the interfacial adhesive energy (φ) on the critical debonding stress with an increased radius of SiO_2 nanoparticles.

4. SUMMARIES

This work examines the influence of adhesive energy on the effective behavior of composites containing nano-sized spherical inclusions. A micromechanics-based framework is derived by incorporating the position dependent Eshelby tensor for a nano-inhomogeneity (Duan et al., 2005) into ensemble volume-averaged method (Ju and Chen, 1994; Yang et al., 2013a). The modified damage model is also adopted into the micromechanical model (Yang et al., 2013a) to predict the effective elastic responses taking into account the particle debonding.

Within the present study, the influences of the adhesive energy between nanoparticle and matrix are examined via numerical simulations. The results indicate that the the interfacial debonding depends on the particle size, and the higher size of nanoparticle leads to lower interface stiffness of the nanocomposites.

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REFERENCES

Duan, H.L., Wang, H.T., Huang, Z.P. and Karihaloo, B.L. (2005), “Eshelby formalism for nano-inhomogeneities”, *P. Roy. Soc. A-Math. Phy.*, 461(1), 3335-3353.

Fu, S.Y., Feng, X.Q., Lauke, B., Mai, Y.W. (2008), "Effects of particle size, particle/matrix interface adhesion and particle loading on mechanical properties of particulate-polymer composites", *Compos. Part B-Eng.*, **39**(6), 933-961.
Ju, J.W., Chen, T.M. (1994), "Micromechanics and effective moduli of elastic composites containing randomly dispersed ellipsoidal inhomogeneities", *Acta. Mech.*, **103**(1-4) 103-121.
Ju, J.W., Lee, H.K. (2000), "A micromechanical damage model for effective elastoplastic behavior of ductile matrix composites considering evolutionary complete particle debonding", *Comput. Method. Appl. M.,* **183**(3-4), 201-222.
Kim, B.R., Pyo, S.H., Lemaire, G., Lee, H.K. (2011), "Multiscale approach to predict the effective elastic behavior of nanoparticle-reinforced polymer composites", *Interaction and Multiscale Mech.*, **4**(3), 173-185.
Odegard G.M., Clancy T.C., Gates T.S. (2005), "Modeling of the mechanical properties of nanoparticle/polymer composites", *Polymer*, **46**(2), 553–62
Weibull, W. (1951), "A statistical distribution function of wide applicability", *J. Appl. Mech.,* **18**(1), 293-297.
Yang, B.J., Shin H., Kim, H., Lee, H.K. (2013a), "Thermo-viscoelastic damage model for nanoparticulate composites by multiscale analysis", in preparation.
Yang, B.J., Shin H., Kim, H., Lee, H.K. (2013b), "A combined molecular dynamics/micromechanics/finite element approach for multiscale constitutive modeling of nanocomposite including interface effect", in preparation.
Yao, X,F., Yeh, H.Y., Zhou, D., Zhang, Y.H. (2006), "The structural characterization and properties of SiO2-epoxy nanocomposites", *J. Compos. Mater.*, **40**(4), 371-381.
Zhang, G., Schlarb, A.K., Tria, S., Elkedim, O. (2008), "Tensile and tribological behaviors of PEEK/nano-SiO2 composites compounded using a ball milling technique", *Compos. Sci. Technol.*, **68**(15-16), 3073-3080.