INVESTIGATING LOCAL PARTICLE AGGREGATION EFFECT ON TENSILE STRENGTH OF COMPOSITES

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Abstract
This research aims to investigate the local aggregation effect on tensile strength of particulate composites with an embedded crack. A micromechanical finite element model (FEM) accounting for the configuration of particle distribution was proposed to study the particle aggregation effect on the fracture behavior of composites. Results reveal that increasing particle size can deteriorate the tensile strength of the composites. The declining behavior would become worse as particle aggregation taking place. Moreover, the decreasing tendency in tensile strength was also observed in the composites with high particle volume fraction in conjunction with high extent of particle aggregation. Therefore, the phenomenon that the particle local aggregation in composites results in the reduction of tensile strength is in a good agreement with experimental observations.

1 Introduction

In past decades, particles in nano-sizes or micro-sizes have been extensively utilized as reinforcement in nanocomposite/composites. However, because of interatomistic interactions, particle aggregation was often observed in the particulate composites/nanocomposites [1-3]. Chen et al. [3] prepared the silica nanocomposites through *in situ* polymerization and blending methods. TEM observation indicates that the samples obtained from *in situ* polymerization demonstrate more homogeneous particle distribution than those prepared from blending methods. In addition, the samples with uniform particle dispersion also exhibit higher tensile strength. Fekete et al. [4] addressed that as the particle size is less than a critical value, the severe particle aggregation would take place resulting in the reduction of tensile strength. Moreover, Evora and Shukla [5] revealed that the particle agglomeration occurring in the samples with volume fraction greater than 1% is responsible for the consistent decrease of tensile strength. The phenomena that as particles size decreases or particle volume fraction increases, the extent of aggregation raises were also reported by Moczo et al [6]. In light of aforementioned investigations, the extent of particles agglomeration is dependent on fabrication process, particle size and volume fraction. Furthermore, when aggregation occurs, the advantage of large surface area diminishes and the corresponding properties of composites are altered. Although the particle aggregation is usually observed in the morphology of composites, its effect on the tensile strength of composites was seldom analyzed in literature. In this study, a micromechanical finite element model (FEM) accounting for different degree of local particle aggregation was generated. The effect particle agglomeration in terms of different particle size and volume fraction was examined from the FEM analysis. The tensile strength of particulate composites was characterized based on the linear elastic fracture mechanics (LEFM) with a crack embedded either within the matrix or in the interface between particle and matrix.

2 Micromechanical Finite Element Model

The finite element micromechanical models as shown in Figure 1 were proposed to simulate the properties of particulate composites containing different degrees of local aggregation. In the finite element models, only the microstructures with local aggregation around the crack are constructed explicitly and the rest area was represented using effective properties. The purpose for generating the embedded model is to save the computer cost since only the stress states near the crack tip in conjunction with the local microstructures are essential to the fracture behavior of the composites. In the microstructure model, except the local aggregation region, the particles were assumed to be distributed uniformly within the matrix. Thus, the corresponding properties for the homogeneous configuration can be represented by the effective material properties calculated from the micromechanics model [7]. Figure 2 illustrates the microstructures of composites with local aggregation in which d is the regular space between the particles and d_{ag} indicates the intra-particle spacing between the two aggregated particles. By adjusting the value of d_{ag} relative to d, the extent of local aggregation was evaluated accordingly. In order to characterize the influence of aggregation on the tensile strength of composites, the crack was embedded either in the matrix or in the interface as shown respectively in Figure 2(a) and Figure 2(b). It is noted that according to our earlier investigation [8], the crack located between the particles as shown in Figure 2(a) is the critical case in predicting the strength of particulate composites. Therefore, the FEM micromechanical model with an embedded crack was employed to demonstrate the aggregation effect on the strength of composites on the basis of linear elastic fracture mechanics (LEFM).

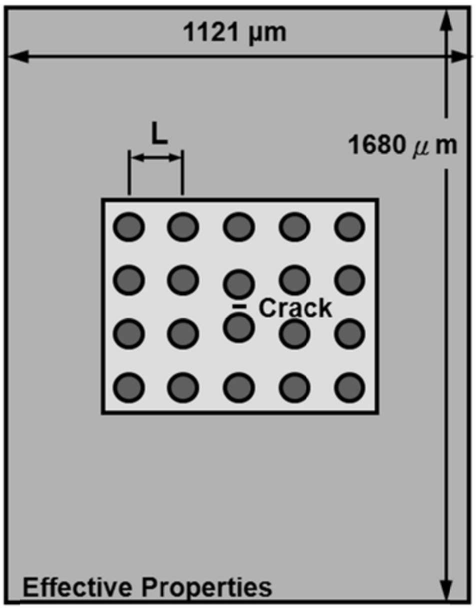

Figure 1. Embedded FEM models for particulate composites with crack (crack length is 2a).

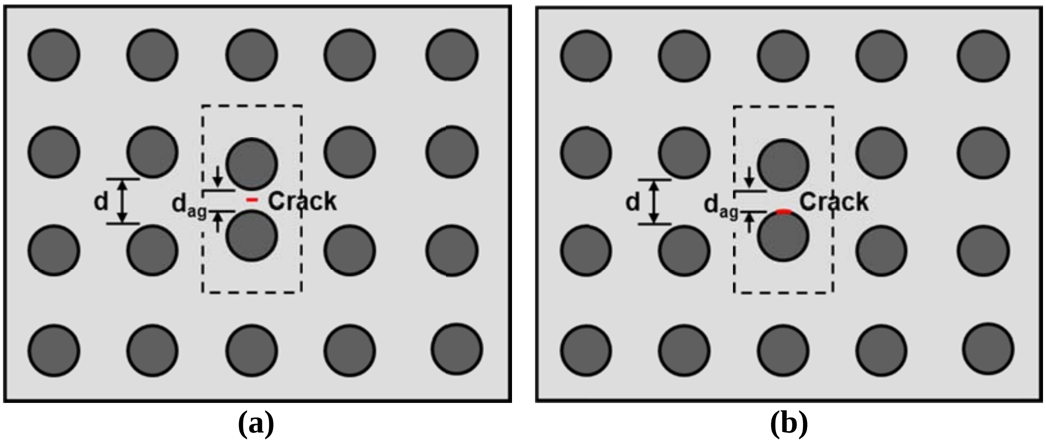

Figure 2. Locations of cracks ((a) within matrix, (b) particle/matrix interface).

3 Linear Elastic Fracture Mechanics

In the theory of LEFM, stress intensity factor (SIF) and strain energy release rate (SERR) are the two parameters generally introduced in modeling the fracture behaviors of continuum solids. Although the two quantities were developed based on different physical concepts (one is from the local stress/displacement filed, and the other is from energy variation), they can be adopted alternatively in predicting the onset of the crack embedded in a continuum solid. In this study, the SERR, due to its simplicity in finite element analysis, was employed to characterize the fracture behaviors of composites. It is noted that in the following analysis, the composites was assumed to be a continuum solid and the particles as well as the surrounding matrix are linear elastic materials. The SERR basically defines the measurement of change in strain energy associated with an infinitesimal crack extension, and when it reaches a critical value, the crack begins to propagate. Irwin [9] proposed a crack closure integral to evaluate the SERR in a cracked solid. By following the same concept, the SERR can also be evaluated using finite element analysis as [10, 11]:

$$G_I = \lim_{\delta a \to 0} \frac{1}{2\delta a}\left[f_y^{p3}(u_y^{p1} - u_y^{p1'}) + f_y^{p4}(u_y^{p2} - u_y^{p2'})\right] \tag{1}$$

$$G_{II} = \lim_{\delta a \to 0} \frac{1}{2\delta a}\left[f_x^{p3}(u_x^{p1} - u_x^{p1'}) + f_x^{p4}(u_x^{p2} - u_x^{p2'})\right] \tag{2}$$

where G_I indicate Mode I SERR and G_{II} represent Mode II SERR. In addition, f_x^{p3} and f_y^{p3} denotes the nodal force at node p_3 in the x and y directions, respectively and f_x^{p4} and f_y^{p4} denotes the nodal force at node p_4 in the x and y direction, respectively. u_x^{p1} and u_y^{p1} are the displacement components at node p_1, and similar definition was applied on nodes p_2, p_1' and p_2' as shown in Figure 3. It is noted the above formulation is derived based on the 8-node 2-D element and the corresponding element size near the crack tip should be at least 1% less than the crack length.

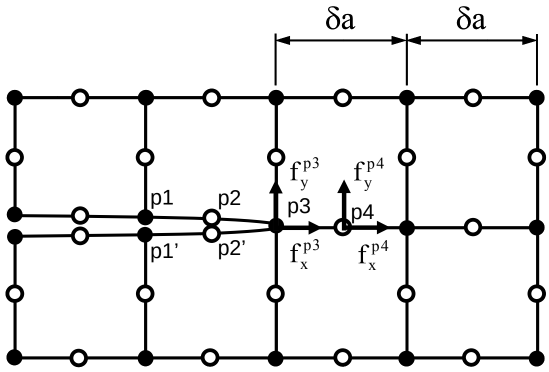

Figure 3. Crack closure method employed in the 8-node 2-D element for finite element analysis.

4 Crack within matrix

4.1 Effect of Particle Size

Figure 4 demonstrates the particle aggregation effect on the tensile strength of the composites in terms of different particle sizes. The obtained values were normalized by the tensile strength in the pure matrix associated with the same crack length. It can be seen that as aggregation increases, the tensile strength decreases. Furthermore, the decreasing tendency is more notable when the agglomerated particles in the composites are larger. As a result, once larger particles are aggregated together, it is possible that the strength of particulate composites would be dramatically decreased.

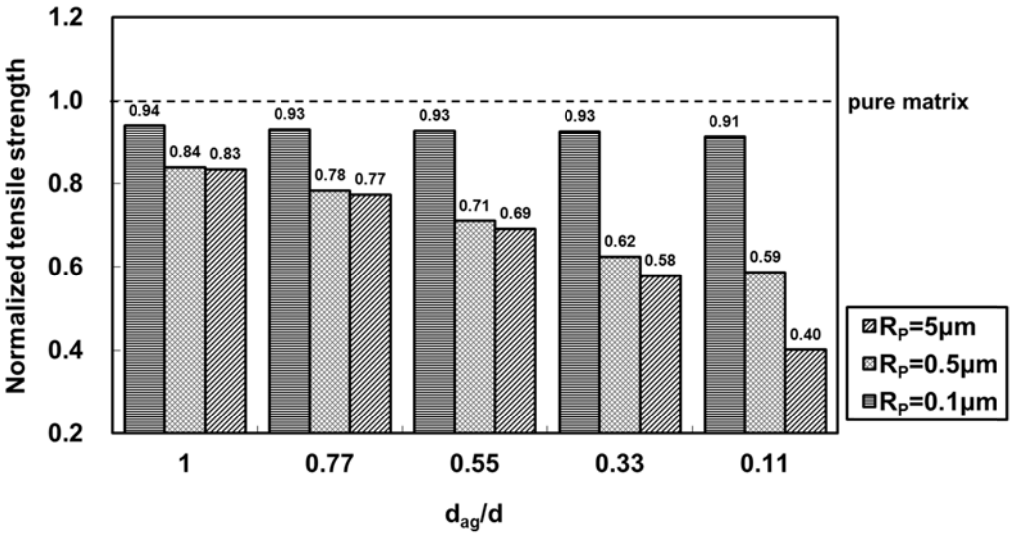

Figure 4. Normalized tensile strength of the nanocomposites with different particle sizes (volume fraction is 10 vol% and half crack length "a" is 0.1 μm).

4.2 Effect of Particle Volume Fraction

In addition to the particle size effect, the influence of particle volume fraction on the tensile strength of composites with different extents of particle aggregation was examined and the results are shown in Figure 5. It is apparent that as the particle volume fraction increases, the normalized tensile strength is decreasing even if the particles are uniformly distributed. Moreover, the increment of particle volume fraction together with particle aggregation would significantly reduce the tensile strength of composites. Such phenomena are quite coincided with the experimental observations [5].

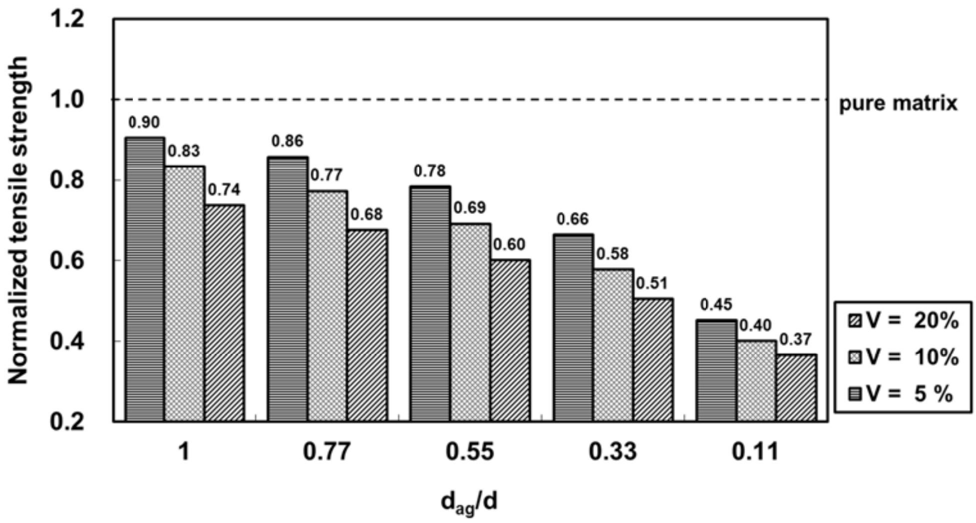

Figure 5. Normalized tensile strength of the nanocomposites with different particle volume fractions (particle size is 5 μm and half crack length "a" is 0.1 μm).

5 Crack on particle/matrix interface

Figure 6 illustrates particle volume effect on tensile strength of composites when the crack is located in the interface between the particle and matrix. Unlike the case where the crack is in matrix, the tensile strength of composite with good particle dispersion is not influenced by volume fraction. Nevertheless, as the degrees of particle aggregation increase, the tensile strength is highly dependent on the volume fraction. In other words, the tensile strength is decreasing with the increment of particle volume fraction. Thus, in order to have better mechanical behaviors, the composites with well dispersed particles should be accomplished during the fabrication process.

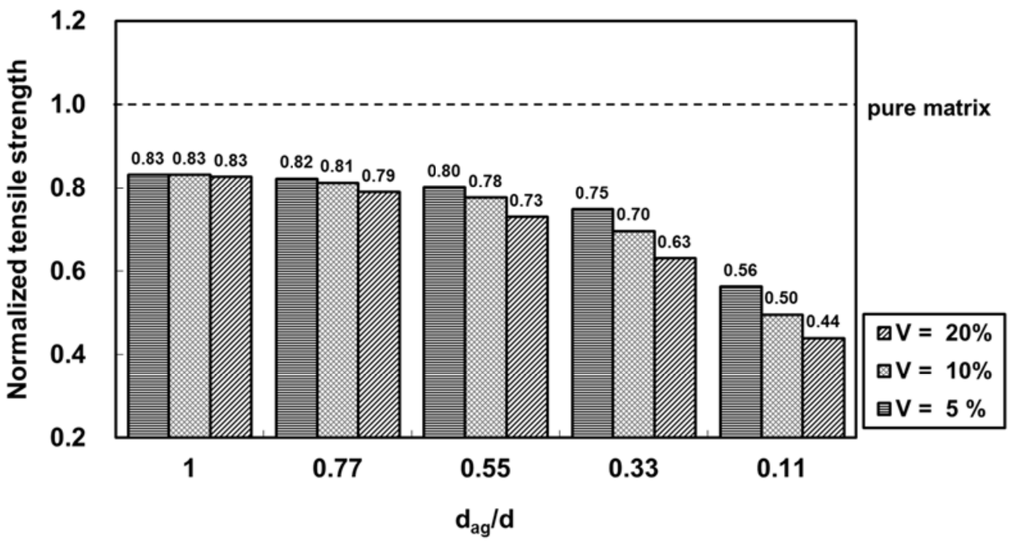

Figure 6. Effect of particle local aggregation on the normalized tensile strength of nanocomposite (particle size is 5 μm and half crack length "a" is 0.1 μm).

6 Summary

In this study, a micromechanical finite element model was developed to characterize the local particle aggregation effect on the tensile strength of composites with an embedded crack.

Results reveal as particle aggregation taking place, the tensile strength of the composites would decrease. The declining behavior would become significant when the particle size is larger or the particle volume fraction is higher. On the other hand, when the initial crack is located in the particle/matrix interface, the tensile strength of composite with good particle dispersion is not influenced by volume fraction. However, when the local aggregation occurs, the reduction rate in tensile strength is raising accompanying with the increment of particle volume fraction. Thus, the local particle aggregation is a critical factor to influence the tensile strength of particulate composites.

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