Analysis of Mechanical Behavior of a Short Fiber Composite Using Micromechanics Based Model*

(Effects of Fiber Clustering on Composite Stiffness and Crack Initiation)

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An injection-molded short fiber composite often contains some fiber clusters due to a poor mixing. An analytical model for a composite with such clusters was developed to estimate a composite stiffness and stresses inside and just outside a fiber of the composite. In this paper, first the stiffness of the cluster is predicted by applying the Eshelby's equivalent inclusion method. Secondly the stiffness of the overall composite and the stress inside a fiber are assessed by applying the Eshelby's method to two kinds of inhomogeneities, i.e. cluster and fiber. Finally the stress just outside the fiber, namely the fiber-end stress, is evaluated using the Hill-Walpole-Mura's jump condition. It is concluded from this parametric study that the effective stiffness of a short fiber composite tends to decrease as the volume fraction of clusters increases, and cracks at fiber ends are more likely to occur at a lower applied stress level as the volume fraction of clusters increases since the magnitude of the fiber-end stress increases. It is found that a carbon fiber composite with higher stiff reinforcement is more sensitive to the negative effects of fiber clustering than a composite with less stiff reinforcement.

Key Words: Cluster, Micromechanics, Injection Molding, Short Fiber Composite, Stiffness, Crack Initiation, Fiber-End Stress

1. Introduction

An injection molding can be used for processing structural components of complicated shape at a moderate cost, while keeping appropriate level of stiffness and strength. However a microstructure in an injection-molded short fiber composite is complicated, and the stiffness and strength are highly dependent on the microstructure. The present authors investigated the effects of thickness ratio, fiber mis-orientation and fiber aspect ratio on the composite

stiffness in the previous paper⁽¹⁾. The effects of inhomogeneous distribution of fibers in a composite on its mechanical behavior have been studied very little.

The injection-molded short fiber composite is generally made of resin matrix with chopped fiber bundles. One fiber bundle consists of several thousands fibers. Thus, under a poor mixing process condition, some fiber clusters would still remain in the resin after injection molding. It is also observed that some fiber clusters would still remain even under a sufficient amount of mixing in case of high volume fractions of fiber⁽²⁾⁻⁽⁴⁾. In this study, the effects of fiber clustering on the stiffness and crack initiations of the injection-molded short fiber composite will be investigated using micromechanics, i.e. the Eshelby's equivalent inclusion method⁽⁵⁾.

2. Analytical Model

2.1 Outline of analytical model

Figure 1 shows an example of a fiber clustering in an injection-molded short fiber composite, shown

* Received 25th August, 1999. Japanese original: Trans. Jpn. Soc. Mech. Eng., Vol. 65, No. 631, A (1999), p. 523-529 (Received 22nd April, 1998)

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Fig. 1 Example of fiber clustering (indicated by arrow)

Fig. 2 Schematic representation of composite with clusters

by the arrow marker. Fibers in the cluster tend to be aligned along the original chopped bundle direction⁽²⁾⁻⁽⁴⁾. Figure 2 schematically illustrates the short fiber composite with some clusters. Firstly the stiffness of the cluster is predicted by applying the Eshelby's equivalent inclusion method⁽⁵⁾ to the cluster. Secondly the composite with clusters as shown in Fig. 2 can be converted to a composite model having two kinds of inhomogeneities⁽⁶⁾, i.e. cluster and fiber as shown in Fig. 3, and the stiffness of the overall composite is assessed by applying the Eshelby's method. Finally the stress inside a fiber is computed, then the stress just outside the fiber, namely the fiber-end stress, is evaluated using the Hill-Walpole-Mura's jump condition.

2.2 Analytical model for a cluster

The analytical model for a cluster consists of an sufficiently large elastic body, namely cluster, containing slightly misoriented short fibers as shown in Fig. 4. The domain of the entire cluster and the fibers are denoted by D_{CL} and Ω , respectively. The stiffness tensors of the matrix and fiber are C_m and C_f , respectively. The fibers are modeled as ellipsoidal inhomogeneities (prolate spheroids) of the same size. It

Fig. 3 Analytical model of short fiber composite with clusters

Fig. 4 Analytical model for a cluster

should be noted that the analytical model is based on the assumptions that both fibers and matrix experience only elastic deformations and that perfect bonding exists at the fiber-matrix interface. The global coordinates are x_1, x_2, x_3 , whereas the local coordinates associated with the fiber are x'_1, x'_2, x'_3 , where x'_3 coincides with the fiber axis, Fig. 4.

Now consider that the composite system is subjected to a uniform applied stress σ_{0CL} . Applying the Eshelby's equivalent inclusion method and Mori-Tanaka's theorem^{(7),(8)} to the model of Fig. 4, the average disturbance of strain $\bar{e}_{CL}$ is related to the strain corresponded to the applied stress e_{0CL} by

$$\bar{e}_{CL} = R \cdot e_{0CL} \quad (1)$$

Furthermore, considering the equivalency of the strain energies of the composite system⁽⁹⁾, the stiffness tensor of the cluster C_{CL} is expressed by

$$C_{CL} = \{[I + Q \cdot (I + R)] \cdot C_m^{-1}\}^{-1} \quad (2)$$

where C_{CL} is a 6×6 matrix and usually anisotropic,

$$R = -[I + P]^{-1} \cdot P \quad (3)$$

$$P = \frac{1}{V_{DCL}} \int_{\Omega} (Z \cdot A \cdot X) dV \quad (4)$$

$$Q = \frac{1}{V_{DCL}} \int_{\Omega} (Z \cdot B \cdot X) dV \quad (5)$$

$$A = (S - I) \cdot B \quad (6)$$

$$B = -[(C_f - C_m) \cdot S + C_m]^{-1} \cdot (C_f - C_m) \quad (7)$$

S is Eshelby's tensor for the fiber in the cluster⁽¹⁰⁾, I is the 6×6 identity matrix, X and Z ($Z \equiv X^{-1}$) are the coordinate transformation matrices and V_{DCL} is the volume of the entire composite, i.e. cluster. P , Q are 6×6 matrices and depend on distribution functions of fiber orientation⁽¹⁾.

2.3 Analytical model for a short fiber composite with clusters

The domain of the analytical model consists of an infinite elastic body containing two kinds of inhomogeneities^{(6),(9)}, i.e. misoriented short fibers and clusters, as shown in Fig. 3. The domain of the entire composite is denoted by D , and the clusters and fibers outside the clusters are denoted by Ω_1 and Ω_2 , respectively. The stiffness tensors of the matrix, cluster and fiber are C_m , C_{CL} (estimated in 2.2) and C_f , respectively. The clusters and fibers are modeled as ellipsoidal inhomogeneities (prolate spheroids) of the same size, where the size of clusters is different from that of the fibers. It should be noted that the analytical model is based on the assumption that the clusters, fibers and matrix experience only elastic deformation and perfect bonding exists at the interface. The global coordinates are x_1, x_2, x_3 , whereas the local coordinates associated with the fiber are x'_1, x'_2, x'_3 and x'_3 is coincident with the fiber axis.

Now consider that the composite system is subjected to a uniform applied stress σ_0 . Applying the Eshelby's method again to this model as shown in Fig. 3, the average disturbance of strain in the matrix $\bar{e}$ is related to the strain corresponded to the applied stress e_0 by

$$\bar{e} = R_{12} \cdot e_0 \quad (8)$$

Furthermore, considering the equivalency of the strain energies of the composite system, the stiffness tensor of the composite C_c (6×6 matrix) is expressed by

$$C_c = [(I + Q_1 \cdot (I + R_{12}) + Q_2 \cdot (I + R_{12})) \cdot C_m^{-1}]^{-1} \quad (9)$$

where

$$R_{12} = -[I + P_1 + P_2]^{-1} \cdot [P_1 + P_2] \quad (10)$$

$$P_1 = \frac{1}{V_D} \int_{\Omega_1} (Z \cdot A_1 \cdot X) dV \quad (11)$$

$$P_2 = \frac{1}{V_D} \int_{\Omega_2} (Z \cdot A_2 \cdot X) dV \quad (12)$$

$$Q_1 = \frac{1}{V_D} \int_{\Omega_1} (Z \cdot B_1 \cdot X) dV \quad (13)$$

$$Q_2 = \frac{1}{V_D} \int_{\Omega_2} (Z \cdot B_2 \cdot X) dV \quad (14)$$

$$A_1 = (S_1 - I) \cdot B_1 \quad (15)$$

$$A_2 = (S_2 - I) \cdot B_2 \quad (16)$$

$$B_1 = -[(C_{CL} - C_m) \cdot S_1 + C_m]^{-1} \cdot (C_{CL} - C_m) \quad (17)$$

$$B_2 = -[(C_f - C_m) \cdot S_2 + C_m]^{-1} \cdot (C_f - C_m) \quad (18)$$

S_1 and S_2 are Eshelby's tensor for the cluster and fiber⁽¹⁰⁾, respectively, I is the 6×6 identity matrix, X and Z ($Z \equiv X^{-1}$) are the coordinate transformation matrices and V_D is the volume of the entire composite. P_1, P_2, Q_1 and Q_2 are 6×6 matrices and depend on distribution functions of fiber orientation.

2.4 Stresses inside and just outside the fiber

A total stress inside a fiber in the cluster σ'_{fCLt} is expressed by :

$$\sigma'_{fCLt} = \sigma'_{0CL} + \sigma'_{fCL} \quad (19)$$

where σ'_{0CL} is the applied stress, σ'_{fCL} is the disturbance stress inside the fiber in the cluster and given by :

$$\sigma'_{fCL} = C_m \cdot [(I + A) \cdot X \cdot \bar{e}_{CL} + A \cdot X \cdot e_{0CL}] \quad (20)$$

' denotes quantities in the local coordinates in Fig. 4. A total stress inside a fiber located outside clusters σ'_{2t} is expressed by :

$$\sigma'_{2t} = \sigma'_0 + \sigma'_2 \quad (21)$$

where σ'_0 is the applied stress, σ'_2 is the disturbance stress inside the fiber located outside clusters and given by :

$$\sigma'_2 = C_m \cdot [(I + A_2) \cdot X \cdot \bar{e} + A_2 \cdot X \cdot e_0] \quad (22)$$

' denotes quantities in the local coordinates in Fig. 3. The following relation holds :

$$\sigma_{0CL} = \sigma'_0 \quad (23)$$

Next the stress just outside the fiber σ^{OUT} can be expressed in terms of the stress inside the fiber σ^{IN} , the stiffness tensors of the matrix C_m and the eigenstrain e^* as follows :^{(5),(11)-(14)}

$$\sigma^{OUT} - \sigma^{IN} = C_m \cdot [-M_n \cdot C_m \cdot e^* + e^*] \quad (24)$$

where

$$M_n = \begin{bmatrix} M_{11}n_1n_1 & M_{12}n_2n_1 & M_{13}n_3n_1 & M_{12}n_3n_1 \\ M_{21}n_1n_2 & M_{22}n_2n_2 & M_{23}n_3n_2 & M_{22}n_3n_2 \\ M_{31}n_1n_3 & M_{32}n_2n_3 & M_{33}n_3n_3 & M_{32}n_3n_3 \\ M_{21}n_1n_3 & M_{22}n_2n_3 & M_{23}n_3n_3 & M_{22}n_3n_3 \\ M_{31}n_1n_1 & M_{32}n_2n_1 & M_{33}n_3n_1 & M_{32}n_3n_1 \\ M_{11}n_1n_2 & M_{12}n_2n_2 & M_{13}n_3n_2 & M_{12}n_3n_2 \\ M_{13}n_1n_1 & M_{11}n_2n_1 \\ M_{23}n_1n_2 & M_{21}n_2n_2 \\ M_{33}n_1n_3 & M_{31}n_2n_3 \\ M_{23}n_1n_3 & M_{21}n_2n_3 \\ M_{33}n_1n_1 & M_{31}n_2n_1 \\ M_{13}n_1n_2 & M_{11}n_2n_2 \end{bmatrix} \quad (25)$$

$$M_{ij} = \frac{1}{G_m} [\delta_{ij} - (n_i n_j) / \{2(1 - \nu_m)\}] \quad (26)$$

G_m and ν_m are the shear modulus and Poisson's ratio of the matrix, δ_{ij} is Kronecker's delta, and n_i is the i -th component of a unit vector outer normal to the inhomogeneity (fiber). This stress just outside the fiber is regarded as the interface stress between fiber and matrix in this paper.

Table 1 Mechanical properties of materials

Material	Young's modulus (GPa)	Poisson's ratio
Poly-Carbonate	2.4	0.38
Carbon Fiber	230.0	0.23
Glass Fiber	72.4	0.22

Fig. 5 Effects of fiber clustering on Young's modulus

3. Results and Discussion

The polycarbonate resin as the matrix and the carbon and glass fibers as the reinforcements are adopted as model materials in this analysis. The mechanical properties of the materials are shown in Table 1.

3.1 Effects of fiber clustering on composite stiffness

The effects of fiber clustering on the effective stiffness of a short fiber composite are investigated by this analytical model. It is assumed that all fibers and clusters are aligned in the x_3 -axis in Fig. 3.

Figure 5 shows the effects of clustering on the Young's modulus in the fiber direction of CF/PC (Carbon Fiber/PolyCarbonate) and GF/PC (Glass Fiber/PolyCarbonate) composites. The horizontal line indicates a fiber volume fraction inside cluster V_{fc} , the vertical line represents the Young's modulus in the fiber direction E_{c3} normalized by the Young's modulus of the matrix E_m and V_{f1} stands for a cluster volume fraction. It is assumed that the aspect ratio of the cluster A_{cl} is 5 and the fiber aspect ratio inside and outside clusters, both A_{fc} and A_{fo} equal to 50. It is noted that the fiber volume fraction outside clusters decreases as the fiber volume fraction inside clusters increases, because the fiber volume fraction of the entire composite V_{fa} is fixed to 0.2.

Figure 5 indicates that the Young's moduli in the fiber direction E_{c3} decreases as the fiber volume frac-

Fig. 6 Effects of fiber clustering on Poisson's ratio

tion inside clusters V_{fc} and the cluster volume fraction V_{f1} increase. It should be noted that the Young's modulus of CF/PC composite in case of $V_{fc}=0.6$ and $V_{f1}=0.2$ decreases to about 60% of that of the composite without clusters. This is attributed to the fact that each fiber in the cluster is too closely distributed to make effective load transfer by shear, while the matrix resin away from the clusters is more likely to deform easily due to the dilute density of fiber. It should be noted that the rate of decrease of the Young's modulus of CF/PC composite, where the stiffness of fiber is higher, is larger than that of GF/PC composite.

Figure 6 shows the effects of clustering on Poisson's ratio of CF/PC and GF/PC composites. The vertical line represents the Poisson's ratio ν_{c23} normalized by the Poisson's ratio of the matrix ν_m and ν_{c23} is the ratio of a compressive strain in the x_3 -direction in Fig. 3 to a tensile strain in the x_2 -direction when a tensile stress is applied in the x_2 -direction. The horizontal line V_{fc} and V_{f1} in Fig. 6 are the same as shown in Fig. 5. $A_{cl}=5$, $A_{fc}=A_{fo}=50$ and V_{fa} is fixed to 0.2 in Fig. 6.

Figure 6 indicates that the Poisson's ratio ν_{c23} increases as the fiber volume fraction in clusters V_{fc} and the cluster volume fraction V_{f1} increase. It is noted that the Poisson's ratio in case of $V_{fc}=0.6$ and $V_{f1}=0.2$ increases to about 1.65 times in CF/PC composite and 1.35 times in GF/PC composite as compared with the composite without clusters. This may be attributed to the same reason as described in Fig. 5, that is, the composite with clusters is more likely to deform in the fiber direction.

The other three independent elastic constants exist in case of the aligned fiber composite. The effects of fiber clustering on these three constants however are found to be little since the rate of change of these constants is less than 3.5% even in the wide range of volume fractions of fibers and clusters.

Fig. 7 Effects of cluster aspect ratio on Young's modulus

Fig. 8 Fiber-end stress for 2-D random composite and aligned fiber composite

Figure 7 shows the effects of cluster aspect ratio A_{cl} on the Young's modulus in the fiber direction as a function of V_{f1} for the case of $V_{fa}=0.2$, $V_{fc}=0.5$, $A_{fc}=A_{fo}=50$. The Young's moduli decrease as the cluster volume fraction V_{f1} increases in case of the cluster aspect ratio A_{cl} being less than about 50. However the Young's modulus changes are very little in case of A_{cl} being more than 50.

3.2 Crack initiation of composite with no cluster

Microcracks occur at the fiber-ends in the direction perpendicular to the fiber axis, if it is aligned along the load direction of a short fiber composite. This phenomenon becomes enhanced more remarkably as the fiber volume fraction is higher, and it was thought that this fiber-end crack contributes to the non-linear portion of the stress-strain relationship of a short fiber composite^{(15),(16)}. It was considered that the fiber-end cracking occurs due to a tensile stress in the fiber direction at the interface between the fiber and matrix at the fiber-ends^{(17),(18)}. Here the crack initiation in a short fiber composite is investigated using the interfacial tensile stress at the pole of the ellipsoidal inhomogeneity, namely a fiber-end stress, computed by using the method described in section 2.4.

Fig. 9 Effects of fiber aspect ratio on fiber-end stress

Only the short fiber composite with no cluster is treated here.

Figure 8 shows the results of fiber-end stress in CF/PC and GF/PC composites with two cases of fiber orientation, aligned and two-dimensional (2-D) random distribution under a tensile stress. The magnitude of the applied tensile stress is 1. The vertical axis represents the fiber-end stress σ_{33}^{OUT} (the interface stress at the pole of the ellipsoidal inhomogeneity), the positive value indicates tensile and the negative one being compressive. The horizontal axis shows the angle θ between the tensile stress direction and the orientation of a fiber. It is assumed that the fiber volume fraction is 0.2 and the fiber aspect ratio is 50.

Figure 8 indicates that the fiber-end stress in a CF/PC composite is a little larger than that in a GF/PC composite, the stress in the aligned case becomes 4 - 5 times larger than the applied stress and the stress in CF/PC and GF/PC composites with 2-D random fiber distribution are about 12 and 9.5 respectively at the fiber-end with $\theta=0$. These indicate high stress concentration at the fiber-end, providing us with further evidence for the microcracks being more likely to occur at the fiber-end first. It is found that the fiber-end crack in the composite with 2-D random fiber distribution begins to occur at a lower applied stress in comparison with the aligned fiber composite, when the fiber volume fraction and fiber aspect ratio are the same for these two composites. Furthermore the fiber-end stress in the composite with 2-D random fiber distribution decreases as the angle θ increases, and the fiber-end stress changes to the compressive side when θ exceeds 60 degrees. The above led us to believe that the fiber-end crack in the composite with random fiber distribution initiates at the fiber which is aligned to the tensile stress direction first and afterward the crack at the misoriented fibers also occurs as the applied stress increases further. These results agree with the experimental data described by Curtis et al⁽¹⁵⁾.

Fig. 10 Effects of cluster in CF/PC on fiber-end stress

Fig. 11 Effects of cluster in GF/PC on fiber-end stress

Figure 9 indicates the fiber-end stress in CF/PC and GF/PC composites as a function of fiber aspect ratio, where the magnitude of the applied tensile stress is 1 and the fiber volume fraction is 0.2.

It follows from Fig. 9 that the fiber-end stress in CF/PC composite is a little larger than that in GF/PC composite, and the fiber-end stress increases with fiber aspect ratio. The rate of this increase slows down when the fiber aspect ratio exceeds 50. The results of Fig. 9 suggests that the fiber-end crack initiated first at relatively long fiber and thereafter the cracks also occur at the shorter fiber as the stress increases. This result also agrees with the experimental observation by Curtis et al.⁽¹⁵⁾

3.3 Effect of clustering on crack initiation

The effects of fiber clustering on the crack initiation are investigated here. It is assumed that all fibers and clusters are aligned in the x_3 -axis, Fig. 3, in order to elucidate the effects of fiber clustering.

Figures 10 and 11 show the computed results of the fiber-end stress in CF/PC and GF/PC composites under the applied stress of 1 as a function of the cluster volume fraction V_{f1} . The effects of the fiber volume fraction inside cluster V_{fc} are also investigated. The solid and broken line in Figs. 10 and 11 show the results of the fiber-end stress at the fibers outside

and inside clusters, respectively. It is assumed that the cluster aspect ratio A_{cl} is 5, the fiber aspect ratios of A_{fc} and A_{fo} are 50. It is noted here that the fiber volume fraction outside clusters decreases as the fiber volume fraction inside clusters increases, since the fiber volume fraction of the entire composite V_{fa} is fixed to 0.2.

The fiber-end stress outside clusters increases as the cluster volume fraction V_{f1} increases when the fiber volume fraction inside clusters V_{fc} remains constant, while the fiber-end stress inside clusters doesn't vary. It is thought that the reason for this is the sharing of load bearing capacity by each fiber outside clusters increases since the fiber volume fraction outside clusters decreases as V_{f1} increases, while that by each fiber inside clusters doesn't vary since the fiber volume fraction inside the cluster V_{fc} is constant. The fiber-end stress outside clusters increases as V_{fc} increases when V_{f1} is constant, however the stress inside clusters decreases. This is due to increasing sharing of load bearing capacity by each fiber outside clusters since the fiber volume fraction outside clusters decreases as V_{fc} increases, while that by each fiber inside clusters decreases since V_{fc} increases. Furthermore the rate of increase of the fiber-end stress in a CF/PC composite is larger than that in a GF/PC composite.

From these results it is considered that the fiber-end cracks are more likely to occur at the fiber outside clusters, contributing to non-linear portion of the stress-strain relationship of a short fiber composite with clusters in comparison to the composite with no cluster. It is found that the effects of fiber clustering in CF/PC composites are more significant than that in GF/PC composites. Furthermore it is important to note that the microcracks (fiber-end cracks) are more likely to occur at fibers not only outside clusters but also inside clusters where the matrix resin doesn't permeate among fibers enough due to a poor mixing.

4. Conclusion

The analytical model for the injection-molded short fiber composite with clusters is developed using the Eshelby's equivalent inclusion method. The effects of fiber clustering on the stiffness and crack initiation are investigated by this model and the following concluding remarks can be obtained:

- (1) The effective stiffness in the fiber direction of the composite decreases as the clusters increase.
- (2) The microcracks at fiber-ends are more likely to occur when the clusters exits in a composite.
- (3) The composite with higher stiff reinforcement such as a carbon fiber is more sensitive to the

negative effects of clustering than that with less stiff reinforcement such as a glass fibers.

(4) Fiber-end cracks in a short fiber composite are more likely to occur first at the fiber of larger aspect ratios and more aligned in the tensile direction, then progressing more at the less aligned fibers. These results agree with the experimental observations.

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