A New Model to Predict Effective Elastic Constants of Composites with Spherical Fillers

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In this study, a new model to predict the effective elastic constants of composites with spherical fillers is proposed. The original Eshelby model is extended to a finite filler volume fraction without using Mori-Tanaka's mean field approach. When single filler is embedded in the matrix, the effective elastic constants of the composite are computed. The composite is in turn considered as a new matrix, where new single filler is again embedded in the matrix. The predicted results by the present model with a series of embedding procedures are compared with those by Mori-Tanaka, self-consistent, and generalized self-consistent models. It is revealed through parametric studies such as stiffness ratio of the filler to the matrix and filler volume fraction that the present model gives more accurate predictions than Mori-Tanaka model without using the complicated numerical scheme used in self-consistent and generalized self-consistent models.

Key Words : Effective Elastic Constants, Eshelby Model, Mori-Tanaka Model, Self-Consistent Model, Generalized Self-Consistent Model, Spherical Filler

Nomenclature

σ_f : Stress in the filler
σ^o : Applied stress
Ω : Fiber domain
$\mathbf{C}_m$: Stiffness of the matrix material
$\mathbf{C}_f$: Stiffness of the filler material
D : Composite domain
$\mathbf{e}^o$: Strain generated in the matrix without the filler by applied stress
$\mathbf{e}$: Strain disturbed by the existence of the filler
$\mathbf{e}^*$: Equivalent eigenstrain of the equivalent inclusion
$\mathbf{e}_c$: Strain generated in the composite by applied stress
E_m : Young's modulus of the matrix
E_f : Young's modulus of the filler
f : Filler volume fraction
$\mathbf{I}$: 6×6 identity matrix
$\mathbf{S}$: Eshelby tensor
$\mathbf{S}_c$: Compliance of the composite
W : Elastic strain energy density

Subscripts

f : The filler
m : The matrix
c : The composite

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1. Introduction

Composites have inherent advantages of their wide range of thermomechanical properties over the unreinforced matrix material, to which much attention has been paid with increasing complicated in-use environment. In order to get the desirable properties of the composites, the composites are designed with the proper selection of constituent materials, filler shape and size, and filler volume fraction, etc. Prior to the design stage, the prediction of the properties by a model is prerequisite through the comprehensive understanding of thermomechanical behavior with variation of parameters. So far many attempts have been made for predicting the effective material properties of composites.

Variational approach has been applied to provide the upper and lower bounds for elastic constants, thermal expansion coefficient, and thermal conductivities of the composites. (Hashin and Shtrikman, 1963) The resulting thermomechanical properties are not exact, but only their range can be guaranteed. For predicting the actual properties of the composites, several models such as the dilute model, the non-dilute model, the self-consistent model, the generalized self-consistent model, and finite element method with a homogenization technique have been introduced. The self-consistent model (SCM) was first proposed to predict the effective elastic constants of composites with spherical fillers, where a single particle is embedded in an infinite matrix of the unknown average properties of the composite. (Budiansky, 1965 ; Hill, 1965) This model is further extended to composites with various shapes of fillers. (Laws and McLaughlin, 1979 ; Chou et al., 1980) Generalized self-consistent model (GSCM) known as a double embedding approach has been applied to composites for the estimation of its material properties. (Christensen and Lo, 1979 ; Dai et al., 1998 ; Dong et al., 2005) This model is widely regarded as superior to other models. (Tucker III and Liang, 1999) In most cases, however, any SCM and GSCM require rigorous numerical computations such as the iterative method. With progress of computer, effective material properties of composites have been predicted by use of the finite element method. (Segurado and Llorca, 2002 ; Saraev and Schmauder, 2003 ; Segurado et al., 2003) Fillers are assumed to be periodically arranged in the matrix and the homogenization technique was employed to compute effective material properties of the composites. Mori-Tanaka model (MTM) has been proposed for predicting the effective material properties of the composites with consideration of interactions between fillers in real composites, which is the modified version of the Eshelby's original method. (Taya and Chou, 1981 ; Taya and Mura, 1981 ; Tandon and Weng, 1984 ; Weng, 1984 ; Lee, 2005 ; Lee and Kim, 2005) It is assumed that each particle sees a far-field strain equal to the average strain in the matrix. Since MTM can be applied to the composites with both periodically and non-periodically arranged fillers, it has been widely used for predicting the effective material properties of the composites due to its relative simplicity and accuracy. (Tucker III and Liang, 1999)

In the present study, the effective elastic constants of composites with spherical fillers are predicted by a new model. The present model (PM) follows faithfully the original Eshelby's equivalent inclusion method to account for the finite volume fraction of fillers instead of using Mori-Tanaka mean field theory for the interactions between fillers. (Eshelby, 1957 ; Mori and Tanaka, 1973) Since Eshelby's original solution only applies to a single particle surrounded by an infinite matrix, it is known that its result is accurate only at low filler volume fraction. Therefore, the effective elastic constants of the composite with a single filler are computed, which is in turn considered as a new matrix material and new single filler is again embedded in it. By repeatedly embedding the filler in the new matrix, the effective elastic constants for the finite volume fraction of fillers are predicted. The results by PM are compared and discussed with those by MTM, SCM, and GSCM for various filler volume fractions and stiffness ratios of the filler to the matrix, through which the applicability of PM is demonstrated.

2. Formulation

Following the Eshelby's equivalent inclusion method to predict the effective elastic constants of the composite, let's consider the composite as single spherical filler embedded in the matrix as shown in Fig. 1(a). (Eshelby, 1957) The original problem is schematically shown in Fig. 1(a), which is converted into the Eshelby's equivalent inclusion problem as shown in Fig. 1(b). $D-\Omega$ and Ω represent the isotropic matrix and filler domains of the composite, respectively, which hereafter are denoted as subscripts m and f, respec-

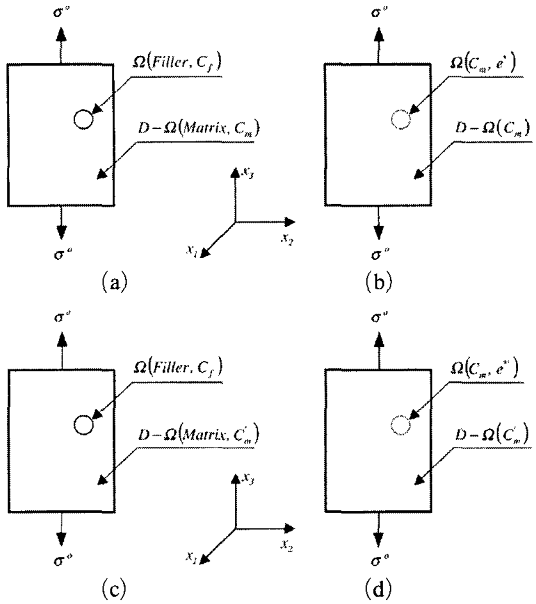


Fig. 1 An analytical model for computing the elastic constants of the composite: (a) Composite with single filler, which is converted to (b) Eshelby's equivalent inclusion problem. (c) Single filler is again embedded in the new matrix, which converted to (d) Eshelby's equivalent inclusion problem

tively. A vector or matrix is represented as a bold-faced letter.

When the composite with the dilute filler is subjected to the uniform stress $\boldsymbol{\sigma}^o$, the stress in the filler and matrix can be determined with the help of Eshelby's equivalent inclusion method. The stress inside the filler $\boldsymbol{\sigma}_f$ can be expressed as

$$\boldsymbol{\sigma}_f=\mathbf{C}_f(\mathbf{e}^o+\mathbf{e})=\mathbf{C}_m(\mathbf{e}^o+\mathbf{e}-\mathbf{e}^*) \qquad (1)$$

where $\mathbf{C}$, $\mathbf{e}$, and $\mathbf{e}^*$ represent the stiffness, the strain disturbed by the existence of the filler, and the equivalent eigenstrain of the equivalent inclusion problem, respectively, and $\mathbf{e}^o$ is related to the applied stress $\boldsymbol{\sigma}^o$ by

$$\boldsymbol{\sigma}^o=\mathbf{C}_m\mathbf{e}^o \qquad (2)$$

The disturbed strain $\mathbf{e}$ in the filler is related through *Eshelby's tensor* $\mathbf{S}$ *as follows:*

$$\mathbf{e}=\mathbf{S}\mathbf{e}^* \qquad (3)$$

where $\mathbf{S}$ is functions of the Poisson's ratio of the matrix and the shape of the filler. From Eqs. (1) ~ (3), the eigenstrain $\mathbf{e}^*$ is explicitly represented as

$$\mathbf{e}^*=-[(\mathbf{C}_f-\mathbf{C}_m)\mathbf{S}+\mathbf{C}_m]^{-1}(\mathbf{C}_f-\mathbf{C}_m)\mathbf{C}_m^{-1}\boldsymbol{\sigma}^o \qquad (4)$$

where $\mathbf{I}$ is 6×6 identity matrix.

Eshelby showed that the elastic strain energy density W of the composite with inhomogeneous inclusions is given by

$$W=\frac{1}{2}\int_D\boldsymbol{\sigma}^o\mathbf{e}^o dv+\frac{1}{2}\int_\Omega\boldsymbol{\sigma}^o\mathbf{e}^* dv \qquad (5)$$

where v denotes the volume to be interated. (Eshelby, 1957)

Since the eigenstrain $\mathbf{e}^*$ is constant in the filler, Eq. (5) can be simply reduced to

$$W=\frac{1}{2}\boldsymbol{\sigma}^o\mathbf{e}^o+\frac{1}{2}f\boldsymbol{\sigma}^o\mathbf{e}^* \qquad (6)$$

where f is the filler volume fraction. The strain energy density of the composite with stiffness $\mathbf{C}_c$ subjected to the uniform applied stress $\boldsymbol{\sigma}^o$ can be expressed as

$$W=\frac{1}{2}\boldsymbol{\sigma}^o\mathbf{e}_c=\frac{1}{2}\boldsymbol{\sigma}^o\mathbf{C}_c^{-1}\boldsymbol{\sigma}^o \qquad (7)$$

Since the elastic strain energy densities computed by both Eq. (6) and (7) must be consistent, Eqs. (4), (6), and (7) is reduced to

$$\boldsymbol{\sigma}^o\mathbf{C}_m^{-1}\boldsymbol{\sigma}^o-f\boldsymbol{\sigma}^o[(\mathbf{C}_f-\mathbf{C}_m)\mathbf{S}+\mathbf{C}_m]^{-1}(\mathbf{C}_f-\mathbf{C}_m)\mathbf{C}_m^{-1}\boldsymbol{\sigma}^o =\boldsymbol{\sigma}^o\mathbf{C}_c^{-1}\boldsymbol{\sigma}^o \qquad (8)$$

Rearranging Eq. (8), the effective stiffness of the composite, $\mathbf{C}_c$, is expressed in explicit form as

$$\mathbf{C}_c=\mathbf{C}_m\{\mathbf{I}-f[(\mathbf{C}_f-\mathbf{C}_m)\mathbf{S}+\mathbf{C}_m]^{-1}(\mathbf{C}_f-\mathbf{C}_m)\}^{-1} \qquad (9)$$

The compliance of the composite is the inverse of the stiffness in Eq. (9), which is given by

$$\mathbf{S}_c=\{\mathbf{I}-f[(\mathbf{C}_f-\mathbf{C}_m)\mathbf{S}+\mathbf{C}_m]^{-1}(\mathbf{C}_f-\mathbf{C}_m)\}\mathbf{C}_m^{-1} \qquad (11)$$

3. Computational Procedures

The present model (PM) is different from the other models such as Mori-Tanaka model (MTM), self-consistent model (SCM), and generalized self-consistent model (GSCM). It is rather more straightforward than SCM and GSCM. The analytical model and schematic representation of computational procedures are shown in detail in Figs. 1 and 2, respectively and their detailed explanations are given as follows.

The model shown in Fig. 1(a) is considered as the composite of the matrix and single filler, based on which Eshelby's equivalent inclusion problem is described in Fig. 1(b). The effective elastic constants of the composite in Fig. 1(a) such as Young's modulus and Poisson's ratio are determined by Eq. (11) derived in the section 2. The composite is considered as the new matrix material, in which an additional filler is embedded as shown Fig. 1(c). Fig. 1(c) is converted into Eshelby's equivalent inclusion problem as shown in Fig. 1(d). Let's assume the initial filler volume fraction in the composite to be f_0 as shown in Fig. 1(c), where the incremental filler volume fraction Δf replaces the composite. With this operation, the removal of filler volume fraction is $f_0\Delta f$, while newly added filler volume fraction is Δf. So, the actual filler volume fraction at this stage is increased to $f_0(1-\Delta f)+\Delta f$ and the actual increase of filler volume fraction is $\Delta f(1-f_0)$. The new effective material properties of the composite are predicted again, which are in turn considered as the new matrix material.

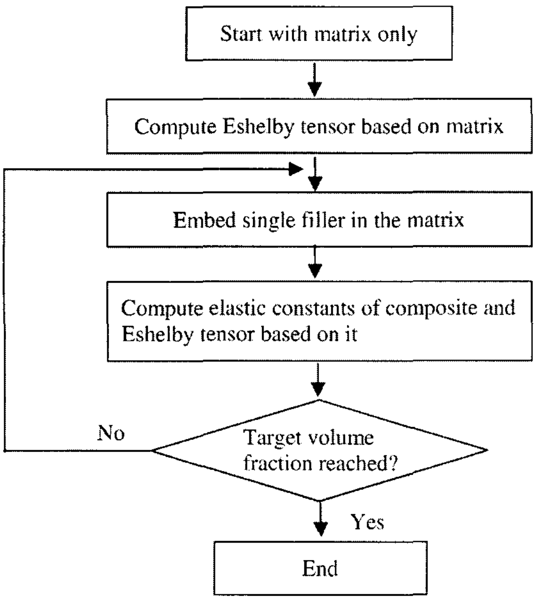


Fig. 2 Schematic representation of the computational procedures used for the present study

Aforementioned procedures are repeated up to the range of the filler volume fraction investigated as shown in Fig. 2.

Table 1 Material properties of the matrix and filler for the present study

	Matrix	Filler
Young's modulus	70 GPa	Variable
Poisson's ratio	0.33	0.165
Aspect ratio	—	1
Volume fraction of fillers	—	Variable

4. Results and Discussions

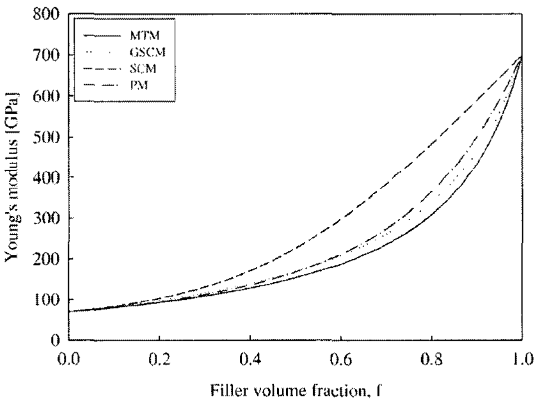
The material properties of the model composite are tabulated in Table 1, which are used for the present study. The Young's modulus and Poisson ratio of the composite with spherical fillers are predicted as a function of filler volume fraction by PM, MTM, SCM, and GSCM. Their results are compared to get the general trend of each model as shown in Fig. 3, where the Young's modulus ratio of the filler to the matrix, E_f/E_m, is kept as 10. The Poisson ratio of the filler is always assumed to be the half of the matrix's one.

According to Fig. 3(a), GSCM predicts a little bit higher Young's modulus of the composite than MTM for the whole f investigated. The difference in predictions between GSCM and MTM is gradually increased with increasing f and it disappears finally at $f=1$. However, the comparison of predictions by both GSCM and PM are quite different. GSCM predicts almost same Young's modulus as PM up to $f=0.55$, beyond which PM predicts higher Young's modulus than GSCM. In similar to the trend of comparison between GSCM and MTM, PM always predicts higher Young's modulus than MTM over the whole f investigated, too. For feasible range of f in real composite world, the predictions by PM are located between GSCM and MTM. It can be roughly concluded that PM predicts more accurately than MTM for the feasible f. As noted in the literature, it is shown that SCM overestimates the Young's modulus over the whole range of f.(Tucker and Liang, 1999) The predictions of

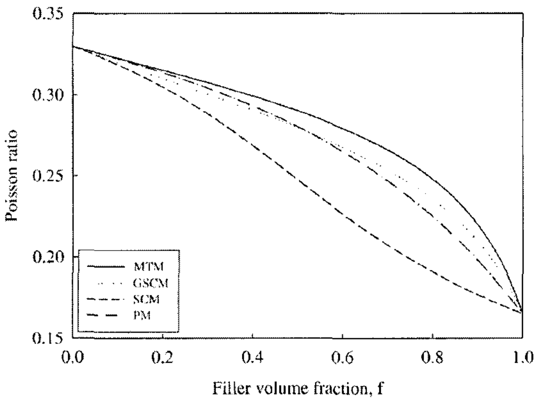
Poisson ratio by the models are shown in Fig. 3 (b), where the results by both GSCM and PM cross each other at $f=0.55$ like the prediction of Young's modulus. It can be stated that the prediction of Poisson ratio by PM shows almost same result as that of Young's modulus. The detailed comparison of the accuracy of the prediction between the models is given below.

In order to examine the accuracy of PM in detail, two parametric studies such as the filler volume fraction and the stiffness ratio E_f/E_m have been made. Since GSCM is generally known to give the best predictions among the models mentioned in introduction, the predicted results by PM and MTM are normalized for an easy comparison by those from GSCM, which are compared and discussed. The filler volume fraction is changed from 0 to 0.6 and stiffness ratio is changed from 5 to 50. The computational results for Young's modulus and Poisson ratio are shown in Fig. 4(a) and (b), respectively.

With the variation of the filler volume fraction and stiffness ratio, the predicted Young's modulus of the composite by PM shows the maximum error of about 8% for $f=0.6$ and E_f/E_m, compared with GSCM. PM predicts Young's modulus within the accuracy of 5% for E_f/E_m of 20 or smaller and the whole f investigated. PM shows

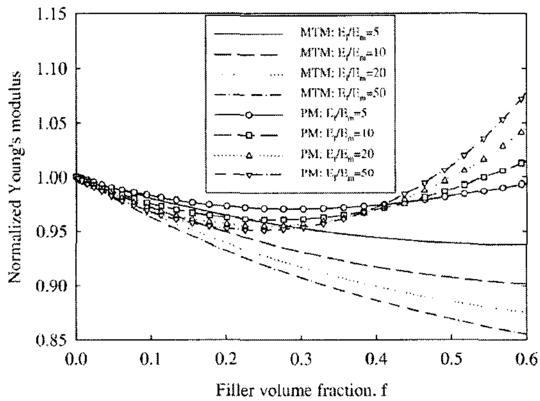


(a) Young's modulus

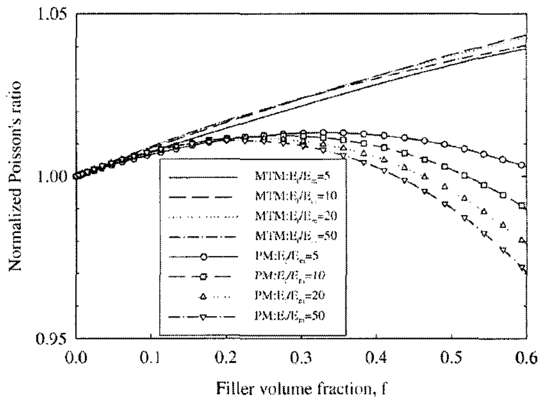


(b) Poisson ratio

Fig. 3 Effective elastic constants of the composite predicted by representative models as a function of filler volume fraction, where Young's modulus and Poisson ratio ratios of the filler to the matrix is kept as 10 and 0.5, respectively



(a) Normalized Young's modulus



(b) Normalized Poisson ratio

Fig. 4 Effective elastic constants of the composite are predicted by PM and MTM and normalized by GSCM as functions of filler volume fraction and stiffness ratio, where the ratio of the Poisson ratio of the filler to that of the matrix is kept as 0.5

the two types of the maximum error such as a local maximum error and the maximum error for a given E_f/E_m. For example, the local maximum errors for E_f/E_m of 5, 10, 20, and 50 take place at $f=0.30$, 0.25, 0.25, and 0.25, respectively. The local maximum error always takes place at low filler volume fraction, which decreases with increasing E_f/E_m to converge at $f=0.25$. The maximum error would take place at $f=0.6$ unless E_f/E_m is smaller than 20. However, the error of MTM increases gradually with increasing f and E_f/E_m, so the local maximum error coincides with the maximum error for f and E_f/E_m investigated. For example, the maximum error is reasonably small for small E_f/E_m of 5, while it reaches about 13% for the largest E_f/E_m of 50.

Comparing PM with MTM, the underestimation of Young's modulus by MTM increases with increasing f and E_f/E_m. The difference between PM and MTM gradually increases from 0 at $f=0$ to the maximum value at around $f=0.5$. For example, the differences between them for E_f/E_m of 50 are about 2, 5, 10, and 12% at $f=0.2$, 0.3, 0.4, and 0.5, respectively. Thus, much attention has been paid to predict the properties of the composite especially for 20~50% filler volume fraction and higher stiffness ratio. Since the computational works by both PM and MTM are nearly same and simple, it is better to use PM rather than MTM in terms of the accuracy.

The predicted Poisson ratios of the composite by both PM and MTM are shown in Fig. 4(b), which are normalized by those from GSCM. Both PM and MTM show reasonably good agreements with GSCM and their errors reaches at most 5% for the given maximum E_f/E_m and f. It can be finally reached that both models can be used for the prediction of Poisson ratio without the loss of accuracy.

5. Conclusions

The new model has been proposed to predict the effective elastic constants of the composites with spherical fillers, where a series of embedding procedures are employed to account for the interactions between the fillers instead of using Mori-Tanaka mean field approach. The present model can predicts accurately both Young's modulus and Poisson ratio of the composite with the filler volume fraction from 0 to 0.6 and stiffness ratio from 5 to 50 within the discrepancies of at most 8% and 3%, respectively. However, Mori-Tanaka model predicts Young's modulus worse than the present model, whose error reaches to about 12% at $f=0.5$ for the stiffness ratio of 50. The Poisson ratio is accurately predicted by this model, and its error is less than 5%. It can be concluded from the present study that the present model is the best choice to predict the effective elastic constants of the composites especially with 20~50% filler volume fraction and higher stiffness ratio in terms of the prediction accuracy and computational cost.

References

Budiansky, B., 1965, "On the Elastic Moduli of Some Heterogeneous Materials," *J. Mech. Phys. Solids*, Vol. 13, pp. 223~227.

Chou, T. W., Nomura S. N. and Taya, M., 1980, "A Self-Consistent Approach to the Elastic Stiffness of Short-Fiber Composites," *J. Comp. Mater.*, Vol. 14, pp. 178~188.

Christensen, R. M. and Lo, K. H., 1979, "Solutions for Effective Shear Properties in Three Phase Sphere and Cylinder Models," *J. Mech. Phys. Solids*, Vol. 27, pp. 315~330.

Dai, L. H., Huang, Z. P. and Wang, R., 1998, "A General Self-Consistent Mori-Tanaka Scheme for Prediction of the Effective Elastic Moduli of Hybrid Multiphase Particulate Composites," *Polymer Composites*, Vol. 19, No. 5, pp. 506~513.

Dong, X. N., Zhang, X., Huang, Y. Y. and Guo, X. E., 2005, "A Generalized Self-Consistent Estimate for the Effective Elastic Moduli of Fiber-Reinforced Composite Materials with Multiple Transversely Isotropic Inclusions," *Int. J. of Mechanical Sciences*, Vol. 47, pp. 922~940.

Eshelby, J. D., 1957, "The Determination of the Elastic Field of an Ellipsoidal Inclusion and Related Problems," *Proc. of the Royal Society of London*, Vol. A241, pp. 376~396.

Hashin, Z. and Shtrikman, S., 1963, "A Variational Approach to the Theory of the Elastic Behavior of Multiphase Materials," *J. Mech. Phys. Solids*, Vol. 11, pp. 127~140.

Hill, R., 1965, "A Self-Consistent Mechanics of Composite Materials," *J. Mech. Phys. Solids*, Vol. 13, pp. 213~222.

Laws, N. and McLaughlin, R., 1979, "The Effect of Fibre Length on the Overall Moduli of Composite Materials," *J. Mech. Phys. Solids*, Vol. 27, pp. 1~13.

Lee, J. K. and Kim, J. G., 2005, "An Analytical Study on Prediction of Effective Elastic Constants of Perforated Plate," *J. Mechanical Science and Technology*, Vol. 19, No. 12, pp. 2224~2230.

Lee, J. K., 2005, "An Analytical Study on Prediction of Effective Properties in Porous and Non-porous Piezoelectric Composites," *J. Mechanical Science and Technology*, Vol. 19, No. 11, pp. 2025~2031.

Mori, T. and Tanaka, K., 1973, "Average Stress in the Matrix and Average Elastic Energy of Materials with Misfitting Inclusions," *Acta Metallurgica*, Vol. 21, pp. 571~574.

Saraev, D. and Schmauder, S., 2003, "Finite Element Modelling of Al/SiCp Metal Matrix Composites with Particles Aligned in Stripes-a 2D-3D Comparison," *Int. J. of Plasticity*, Vol. 19, pp. 733~747.

Segurado, J. and Llorca, J., 2002, "A Numerical Approximation to the Elastic Properties of Sphere-reinforced Composites," *J. Mech. Phys. Solids*, Vol. 50, pp. 2107~2121.

Segurado, J., Gonzalez, C. and Llorca, J., 2003, "A numerical Investigation of the effect of Particle Clustering on the Mechanical Properties of Composites," Acta Materialia, Vol. 51, pp. 2355~2369.

Tandon, G. P. and Weng, G. J., 1984, "The Effect of Aspect Ratio of Inclusions on the Elastic Properties of Unidirectionally Aligned Composites," *Polymer Composites*, Vol. 5, pp. 327~333.

Taya, M. and Arsenault, R. J., 1987, "Metal Matrix Composites-Thermomechanical Behavior," *Pergamon Press*, pp. 35~36.

Taya, M. and Chou, T. W., 1981, "On two Kinds of Ellipsoidal Inhomogeneities in an Infinite Elastic Bodey : an Application to a Hybrid Composite," *Int. J. Solids Structures*, Vol. 17, pp. 553~563.

Taya, M. and Mura, T., 1981, "On Stiffness and Strength of an Aligned Short-Fiber Reinforced Composite Containing Fiber-End cracks Under Uni-Axial Apllied Stress," *ASME J Applied Mech.*, Vol. 48, pp. 361~367.

Tucker III, C. L. and Liang, E., 1999, "Stiffness Predictions for Unidirectional Short-Fiber Composites : Review and Evaluation," *Composites Science and Technology*, Vol. 59, pp. 655~671.

Weng, G. J., 1984, "Some Elastic Properties of Reinforced Solids, with Special Reference to Isotropic Ones Containing Spherical Inclusions," *Int. J. Engineering Science*, Vol. 22, pp. 845~856.