PERGAMON

International Journal of Solids and Structures 39 (2002) 649–657

INTERNATIONAL JOURNAL OF SOLIDS and STRUCTURES

www.elsevier.com/locate/ijsolstr

A modified model for the prediction of effective elastic moduli of composite materials

Pin Lu [a,b,*], K.H. Lee [a]

[a] Institute of High Performance Computing, 89C Science Park Drive, #02-11/12 The Rutherford, Singapore 118261

[b] Department of Modern Mechanics, University of Science and Technology of China, Hefei, Anhui 230026, China

Received 17 August 2000

Abstract

In the present paper, the procedure for successive iteration method proposed by Mori and Wakashima [Micromechanics and Inhomogeneity, 1990] to estimate the effective elastic moduli of composite materials is reviewed. It is observed that the formulations of the method could be modified and generalized by introducing a parameter called concentration factor in the expression of the equivalent eigenstrain. The concentration factor introduced reflects the approximation to the interaction among the reinforcing particles in a composite. With the proper choice of the concentration factor, the dilute and Mori–Tanaka models can be obtained as the specific cases of the modified formulations. The properties of the concentration factor are discussed. Numerical examples show a way to determine the factor through known experimental or numerical results of the considered problems. © 2002 Elsevier Science Ltd. All rights reserved.

Keywords: Effective elastic moduli; Composite materials; Successive iteration method

1. Introduction

Prediction and estimation of effective elastic properties of composite materials with inclusions are of great interest to researchers and engineers in many science and engineering disciplines. In dealing with how the material properties of each component and microgeometry influence the overall response of composite materials, a number of approximate approaches have been proposed in literature. Those received most attention are dilute, Mori–Tanaka, self-consistent and differential schemes (Mura, 1987; Aboudi, 1991). Based on the concept of stress and strain concentration matrix (Benveniste, 1987), these methods can be expressed in a unified form (Dunn and Taya, 1993), in which only the concentration matrices have different expressions for the different prediction models. These concentration matrices are obtained through various

* Corresponding author. Address: Institute of High Performance Computing, 89C Science Park Drive, #02-11/12 The Rutherford, Singapore 118261. Tel.: +0065-874-8934.

E-mail address: mpelup@nus.edu.sg (P. Lu).

PII: S0020-7683(01)00162-7

approximations. As it is known, the interaction between the inhomogeneous inclusions is an open problem and its analytical solution is virtually impossible. The various interaction models in literature, despite based on rigorous mathematical derivations, are still approximate predications and are usually only applicable to specific cases. Therefore, improving existed models based on some physical analysis may offer a simple but effective way to construct satisfied predicating models. The present work tries to make an attempt in this way.

In the paper of Mori and Wakashima (1990), a successive iteration method was proposed to evaluate the stress and strain disturbances due to inhomogeneities in a composite. The method offers a physical basis of the average field approach. By investigating the process and physical relations of the method, it is observed that the formulations of the method could be extended to get a more general model. In the present paper, some properties in the successive iteration method are discussed. A concept called concentration factor is introduced into the theoretical framework, which reflects the influence of the interactions between inhomogeneities. In general, the introduced concentration factor is the function of phase volume fraction and shapes of the inhomogeneities. For a considered composite material, it could be determined through the known properties of the material such as experimental data and numerical results etc. By introducing the concentration factor, a modified model to predict the overall properties of materials is provided. It could be considered as an extension of the formulations obtained by the successive iteration method.

In the next section, the successive iteration method is briefly reviewed. The improved treatment is then discussed in Section 3 and the examples of two-phase elastic composites with randomly distributed elastic spheres are given in Section 4 to show the validity of the modified prediction model.

2. Successive iteration method and modification

Consider a body, D, which consists of a matrix and a large number of randomly distributed ellipsoidal inhomogeneities Ω. The elastic stiffnesses of the matrix and inhomogeneities are $\mathbf{C}$ and $\mathbf{C}^*$, respectively. Let the displacement at the boundary of the body is prescribed. The prescribed displacement produces a uniform strain γ_0 and stress σ_0 in the homogeneous body without containing the inhomogeneities:

$$\sigma_0 = \mathbf{C}\gamma_0, \qquad \gamma_0 = \mathbf{C}^{-1}\sigma_0. \tag{1}$$

Since the body contains the inhomogeneities, the strain changes to $\gamma_0 + \gamma$ and the stress to $\sigma_0 + \sigma$. The terms γ and σ are called disturbances due to the presence of the inhomogeneities. Since the strain is prescribed, the average of the disturbed strain must vanish (Mura, 1987), i.e.

$$f\langle\gamma\rangle_\Omega + (1-f)\langle\gamma\rangle_{\mathrm{M}} = 0, \tag{2}$$

where $\langle\cdot\rangle_\Omega$ and $\langle\cdot\rangle_{\mathrm{M}}$ denote the averages of relevant quantities over the inhomogeneities and matrix, respectively, and f is the volume fraction of the inhomogeneities. The average fields $\langle\gamma\rangle_{\mathrm{M}}$, $\langle\gamma\rangle_\Omega$ as well as $\langle\sigma\rangle_{\mathrm{M}}$ and $\langle\sigma\rangle_\Omega$ can be obtained from relation (2) and equivalent inclusion method (Mura, 1987). They are solved as

$$\langle\gamma\rangle_{\mathrm{M}} = -f\mathbf{S}\varepsilon^*, \qquad \langle\gamma\rangle_\Omega = (1-f)\mathbf{S}\varepsilon^* \tag{3}$$

and

$$\langle\sigma\rangle_{\mathrm{M}} = \mathbf{C}\langle\gamma\rangle_{\mathrm{M}}, \qquad \langle\sigma\rangle_\Omega = \mathbf{C}(\langle\gamma\rangle_{\mathrm{M}} - \varepsilon^*), \tag{4}$$

where $\mathbf{S}$ is Eshelby tensor for the equivalent inclusion, Eshelby (1957), and ε^* is the equivalent eigenstrains. It is seen that as soon as the equivalent eigenstrains ε^* is determined properly, the average fields and overall elastic constants of the composite are readily obtained.

The successive iteration method therefore provides an approximate procedure to evaluate ε^* as well as average fields. The method consists of the following procedures: The stress disturbance in a single representative inhomogeneity is evaluated at first. Then, the contribution of the other inhomogeneities is taken into account by considering that the representative inhomogeneity feels the additional field by the other inhomogeneities. These processes are repeated. In this way, the equivalent eigenstrains ε^* can be obtained in series form as

$$\varepsilon^* = \varepsilon_0^* + \varepsilon_1^* + \varepsilon_2^* + \cdots, \tag{5}$$

where

$$\varepsilon_i^* = -f\mathbf{B}\varepsilon_{i-1}^* \tag{6}$$

and

$$\mathbf{B} = \mathbf{Z}^{-1}(\mathbf{C} - \mathbf{C}^*)\mathbf{S}, \qquad \mathbf{Z} = (\mathbf{C}^* - \mathbf{C})\mathbf{S} + \mathbf{C}. \tag{7}$$

When the magnitude of every eigenvalue of $-f\mathbf{B}$ is less than one, and the correction procedures are repeated infinite times, the series (5) converges to the expression of

$$\varepsilon^* = (\mathbf{I} + f\mathbf{B})^{-1}\varepsilon_0^* \tag{8}$$

after substitution of the relation (6). Here ε_0^* is the equivalent eigenstrain when only a single inhomogeneity is considered, and is obtained as

$$\varepsilon_0^* = \mathbf{Z}^{-1}(\mathbf{C} - \mathbf{C}^*)\gamma_0. \tag{9}$$

It is seen that the successive iteration method is a repeating process to obtain the approximate equivalent eigenstrains ε^* given in Eqs. (5)–(9) and (6) is the fundamental relation of the approach. Based on the relation, the limiting case of the successive iteration method is found equivalent to the Mori–Tanaka model. It means that under the approximation of Eq. (6), the successive iteration method can only reach the accuracy of the Mori–Tanaka method at most. Therefore, one might intuitively argue that a correction factor corresponding to but differing from $-f\mathbf{B}$ in Eq. (6) can be used so that the successive iteration method can provide better predictions. It was pointed out but was not discussed further by Mori and Wakashima (1990). To do so, the correction factor in Eq. (6) could be modified as

$$\varepsilon_i^* = -\beta\mathbf{B}\varepsilon_{i-1}^* \tag{10}$$

in which the volume fraction of the inclusions in Eq. (6) is replaced by a generalized parameter β. It is noted that the modified relation (10) is introduced to have similar form as Eq. (6). It is to ensure that the overall stiffness obtained through the relation is still the inverse of the overall compliance. Although Eq. (10) has a similar form as Eq. (6), expression (10) has a more general physic meaning. Generally, the analytical form of β cannot be obtained because the interactions between inhomogeneities are very complicated. Since β is basically the function of volume fraction, inhomogeneity shapes and other material properties for a considered problem, Eq. (10) provides a way to improve the approximations by optimizing the parameter β. By setting $\beta = f$, the relation (10) returns to the conventional expression (6). Therefore, Eq. (10) can be considered as the generalization of Eq. (6). Furthermore, Eq. (8) can be written as

$$\varepsilon^* = (\mathbf{I} + \beta\mathbf{B})^{-1}\varepsilon_0^*. \tag{11}$$

With the modified relations (10) and (11), the average stress disturbances $\langle\sigma\rangle_{\mathrm{M}}$ and $\langle\sigma\rangle_{\Omega}$ in the matrix and inhomogeneities are obtained by substituting Eqs. (3) and (11) into Eq. (4), respectively, as

$$\langle\sigma\rangle_{\mathrm{M}} = -f\mathbf{C}\mathbf{S}(\mathbf{I} + \beta\mathbf{B})^{-1}\varepsilon_0^*, \qquad \langle\sigma\rangle_{\Omega} = \mathbf{C}[(1-f)\mathbf{S} - \mathbf{I}](\mathbf{I} + \beta\mathbf{B})^{-1}\varepsilon_0^*. \tag{12}$$

Furthermore, the average stress disturbance over the body is given by

$$\langle\sigma\rangle = f\langle\sigma\rangle_{\Omega} + (1-f)\langle\sigma\rangle_{M}. \tag{13}$$

Substitution of Eqs. (9) and (12) into Eq. (13) yields

$$\langle\sigma\rangle = -f\mathbf{C}(\mathbf{I}+\beta\mathbf{B})^{-1}\mathbf{Z}^{-1}(\mathbf{C}-\mathbf{C}^{*})\gamma_0. \tag{14}$$

3. Modified model for prediction of effective elastic moduli

Following the discussion of the last section, the average stress, $\overline{\sigma}$, over the body is defined by

$$\overline{\sigma} = \overline{\mathbf{C}}\overline{\gamma}, \tag{15}$$

where $\overline{\mathbf{C}}$ is overall elastic moduli and $\bar{\gamma} = \gamma_0$ by the average strain theorem (Aboudi, 1991). According to the definition, the above average stress can be written as

$$\overline{\mathbf{C}}\gamma_0 = \mathbf{C}\gamma_0 + \langle\sigma\rangle. \tag{16}$$

By using the relation (14), the overall elastic moduli, $\overline{\mathbf{C}}$, is obtained as

$$\overline{\mathbf{C}} = \mathbf{C}\{\mathbf{I} + f[(1-\beta)(\mathbf{C}^{*}-\mathbf{C})\mathbf{S}+\mathbf{C}]^{-1}(\mathbf{C}^{*}-\mathbf{C})\}. \tag{17}$$

It is seen that some of commonly used prediction models can be derived from the above expression. To show it, we write out the explicit expressions of the dilute and Mori–Tanaka models as

$$\overline{\mathbf{C}}^{\mathrm{dil}} = \mathbf{C}\{\mathbf{I} + f[(\mathbf{C}^{*}-\mathbf{C})\mathbf{S}+\mathbf{C}]^{-1}(\mathbf{C}^{*}-\mathbf{C})\}, \tag{18}$$

$$\overline{\mathbf{C}}^{\mathrm{M–T}} = \mathbf{C}\{\mathbf{I} + f[(1-f)(\mathbf{C}^{*}-\mathbf{C})\mathbf{S}+\mathbf{C}]^{-1}(\mathbf{C}^{*}-\mathbf{C})\}, \tag{19}$$

where the superscripts dil and M–T indicate dilute and Mori–Tanaka models, respectively. It is seen that the expression (17) is reduced to the dilute and the Mori–Tanaka models, respectively, when the parameter β is chosen to be zero and f, respectively. This indicates that β is indeed a parameter to influence the prediction results. By changing the parameter, different models can be obtained. With proper optimization of β, one could attain better prediction results. Therefore, the parameter β is introduced on the physical basis. With the modification, the formulations of the successive iteration method are extended to more general cases.

Defining the concentration factor α to be

$$\alpha = 1-\beta, \tag{20}$$

Eq. (17) can be written in a more concise form as

$$\overline{\mathbf{C}} = \mathbf{C}\{\mathbf{I} + f[\alpha(\mathbf{C}^{*}-\mathbf{C})\mathbf{S}+\mathbf{C}]^{-1}(\mathbf{C}^{*}-\mathbf{C})\}. \tag{21}$$

Same as the parameter β, the concentration factor α is also a parameter reflecting the influence of the interaction among the inhomogeneities, and generally depends on many variables, such as volume fractions, shapes of the inhomogeneities, material properties of both matrix and inhomogeneities etc. Due to the complexity of a real problem, it is impossible to obtain a general analytical form of α through mathematical derivations.

Unlike most of existed prediction models, the expression (17) or (20) contains an unfixed parameter. It makes the formulation more *adjustable*. One can determine the parameter approximately based on some known information of considered materials, such as numerical and experimental results etc. In this way, some properties of the composite can be well included, which may be omitted through various assumptions or could not be considered well due to the restriction of mathematical treatments. Although a large amount of prediction models and methods by using micromechanics and mathematical derivations have been reported in the literature, none of them is universal applicable. Since some properties, such as interactions among inhomogeneities etc., are impossible to be clearly described analytically, every theory prediction method is virtually based on some specific assumptions and approximations, and hence has lost some useful information. This will certainly influence prediction accuracy. To capture the lost information, which could not be obtained by analytical method, in certain degree, some parameters can be introduced into the theory model and are determined through some known material properties. In this way, the modified model should be improved. Therefore, it is a simple but effective treatment to improve the prediction results.

If the influence of volume fraction f is considered only for simplicity, the concentration factor α can be expressed in the function of f. By examining Eq. (21), it is found that α should equal zero if the body is fully filled by the inhomogeneities. Therefore, in polynomial the concentration factor α may have the form

$$\alpha = (1 - f)(1 + \alpha_1 f + \alpha_2 f^2 + \alpha_3 f^3 + \cdots), \tag{22}$$

where $\alpha_1, \alpha_2, \alpha_3, \ldots$, are coefficients, which can be determined through the known information of the considered materials. By setting $\alpha_1 = \alpha_2 = \cdots = 0$, Eq. (22) is reduced to the approximation for Mori–Tanaka model, which is also the limiting case of the successive iteration method under the approximation of the relation (6). Therefore, Eq. (21) could be considered as a generalization of the expression derived from of the successive iteration method.

4. Examples and discussion

As indicated before, the concentration factor can be obtained through some known information of considered materials. In this section, we show a treatment to determine the concentration factor according to available experiment data. As examples, the experimental data for the materials of two-phase elastic composites with randomly distributed elastic spheres, recorded by Smith (1976) and Richard (1975), are used here. The material properties involved in these two experiments are: (i) $E = 3$ GPa, $v = 0.4$, $E^* = 76$ GPa and $v^* = 0.23$ from Smith's data; (ii) $E = 1.69$ GPa ($= 2.45 \times 10^5$ psi), $v = 0.444$, $E^* = 70.33$ GPa ($= 102 \times 10^5$ psi) and $v^* = 0.21$ from Richard's data. Here, E and v are the Young's modulus and Poisson's ratio of the matrix, respectively; E^* and v^* are ones of the spherical inhomogeneities.

The relationships between the general elastic stiffnesses C_{ijkl} and the material constants E and v are given by (Aboudi, 1991):

$$C_{ijkl} = \frac{Ev}{(1+v)(1-2v)}\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{23}$$

where

$$\mu = \frac{E}{2(1+v)} \tag{24}$$

is shear modulus and δ_{ij} is the Kronecker delta. Based on Eq. (23), the Eshelby tensor $\mathbf{S}$ for a spherical isotropic inclusion can be written as (Mura, 1987)

$$\begin{aligned} &S_{1111} = S_{2222} = S_{3333} = \frac{7-5v^*}{15(1-v^*)}, \quad S_{1212} = S_{2323} = S_{3131} = \frac{4-5v^*}{15(1-v^*)}, \\ &S_{1122} = S_{2233} = S_{3311} = S_{1133} = S_{2211} = S_{3322} = \frac{5v^*-1}{15(1-v^*)}. \end{aligned} \tag{25}$$

The experimental data by Smith (1976) are listed in Table 1, in which f is the volume fraction of the spherical inhomogeneities, $\overline{E}$ the overall Young's modulus, μ and $\bar{\mu}$ are the matrix and the overall shear

Table 1
Experimental data recorded by Smith (1976)

f	0	0.1	0.225	0.3	0.398	0.495
$\overline{E}$(GPa)	3	3.75	5.1	6	7.9	12.1
$\bar{\mu}/\mu$	1	1.25	1.7	2	2.67	4.12

Table 2
Approximate results calculated from Eq. (27)

f	0	0.1	0.225	0.3	0.398	0.495
α	1	0.8	0.625	0.565	0.445	0.265

modulus, respectively. Since only the effect of volume fraction is taken to be variable in the experimental data of Table 1, the concentration factor can be written in the form of Eq. (22). According to Table 1, the values of the concentration factor α at the known data of volume fractions and overall properties can be determined by solving Eq. (21):

$$\alpha = [f(\mathbf{C}^* - \mathbf{C})(\mathbf{C}^{-1}\overline{\mathbf{C}} - \mathbf{I})^{-1} - \mathbf{C}]\mathbf{S}^{-1}(\mathbf{C}^* - \mathbf{C})^{-1}. \tag{26}$$

The calculated results based on the data in Table 1 are listed in Table 2.

By using the results of f and α listed in Table 2, the coefficients in Eq. (22) can be determined. If only three terms of the polynomial are considered, the coefficients α_1, α_2 and α_3 can be determined according to three groups of values f and α in Table 2. Taking, for example, $f = 0.1$, 0.3, 0.495 and corresponding $\alpha = 0.8$, 0.565, 0.265 respectively, the coefficients α_1, α_2 and α_3 are obtained by substituting the relevant f and α into Eq. (22): $\alpha_1 = -1.64662$, $\alpha_2 = 6.95964$, $\alpha_3 = -10.04591$. Therefore, the approximate concentration factor α for this problem can be obtained as

$$\alpha = (1 - f)(1 - 1.64662f + 6.95964f^2 - 10.04591f^3). \tag{27}$$

Fig. 1 shows the comparison of the concentration factors α for different prediction models. It can be seen that the curve by including the information of the experimental results is lower than that of Mori–Tanaka model for this problem, and the relation $0 \leqslant \alpha \leqslant 1$ exists for all cases. Figs. 2 and 3 show the predictions of the effective Young's modulus $\overline{E}$ and effective shear modulus $\bar{\mu}$ versus volume fraction f according to different models. The experimental data were recorded by Smith (1976). It is observed that the agreement

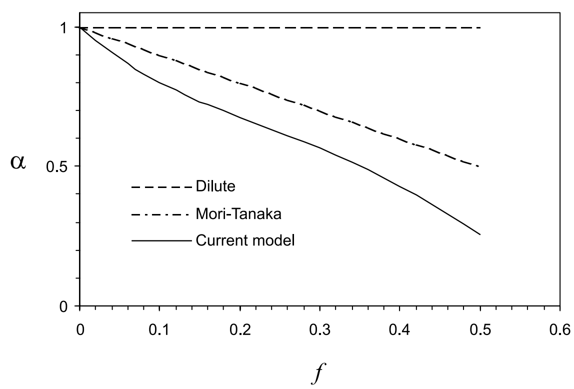

Fig. 1. Comparison of the concentration factors α for the different micromechanical models.

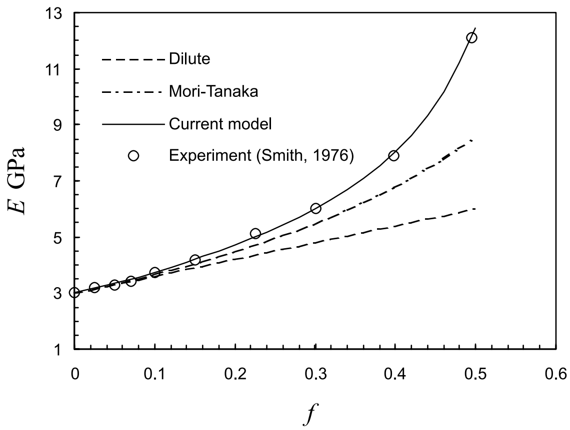

Fig. 2. Comparison of the micromechanical predictions and the experimental results by Smith (1976) for the effective Young's modulus $\overline{E}$ as a function of particle volume fraction.

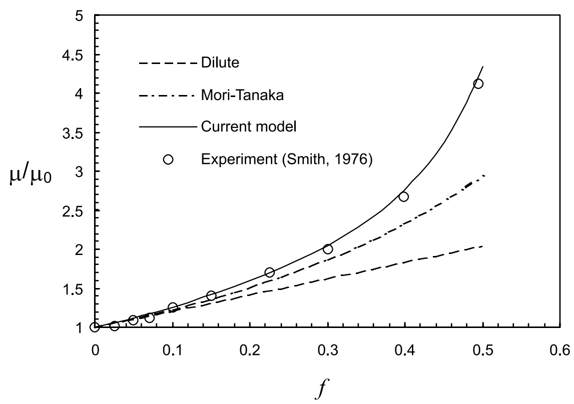

Fig. 3. Comparison of the micromechanical predictions and the experimental results by Smith (1976) for the effective shear modulus $\bar{\mu}$ as a function of particle volume fraction.

between the predictions of the modified model and experimental data is very good for both effective Young's modulus and effective shear modulus. It is due to the reason that the concentration factor α for the modified model is improved according to the known experimental data of the materials. Therefore, some properties of the composite are included. It should be pointed out that it is not just a simple curve fitting. With the modification, some matrix/inclusion interaction and microstructure properties of the composites with similar material systems, which are unable to be described by mathematical models but may be captured by the information of experimental results, can be included into the modified model. In case that theory model could not provide ideal prediction, a modification according to known results is a reasonable alternative choice.

Generally, the concentration factor α should vary with material properties, shapes of inhomogeneities etc. Therefore, α are different for different problems. However, for the composites with similar material system and structures, i.e. same phase number and microgeometry of inhomogeneities etc., related concentration factors should be similar. To verify the deduction, the approximate concentration factor (27), which is obtained according to the experimental data of the material used by Smith (1976), is used to

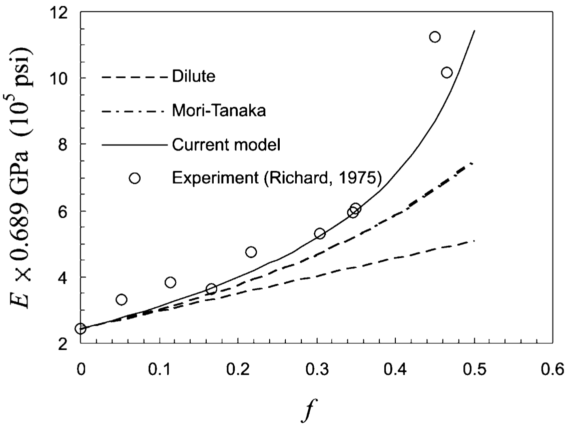

Fig. 4. Comparison of the micromechanical predictions and the experimental results by Richard (1975) for the effective Young's modulus $\overline{E}$ as a function of particle volume fraction.

predict the overall properties of another composite material used by Richard (1975). As described, these two materials have similar structures, two-phase elastic composites with randomly distributed elastic spheres. Fig. 4 shows the prediction results. It is seen that with the concentration factor (27), the modified model still can provide a much better prediction than those by Mori–Tanaka and dilute models. This example provides a support on the above deduction. For different material systems, however, care should be taken because the material properties included in the concentration factor for one material system may not suitable for other material systems.

5. Concluding remarks

By examining the procedure of the successive iteration method, a modified model is suggested to predicate effective properties of composite material containing randomly dispersed inhomogeneities. The modified model can be considered to be a generalization of the formulations of the successive iteration method. In the modified model, the parameter called concentration factor is introduced on the physical basis. Since the concentration factor can be determined through the experimental data and some other useful information of considered material, the modified model can provide a better prediction. For further work, the properties of the concentration factor α should be investigated.

The method used in this paper is an alternative attempt to construct modified prediction models. Some concepts and basic treatments are introduced. To have the method more applicable, there are still some problems to be solved.

References

Aboudi, J., 1991. Mechanics of Composite Materials. Elsevier, Amsterdam.
Benveniste, Y., 1987. A new approach to the application of Mori–Tanaka's theory in composite materials. Mech. Mater. 6, 147–157.
Dunn, M.L., Taya, M., 1993. Micromechanics predictions of the effective electroelastic moduli of piezoelectric composites. Int. J. Solids Struct. 30, 161–175.

Eshelby, J.D., 1957. The determination of the elastic field of an ellipsoidal inclusion and related problems. Proc. Roy. Soc. London A241, 376–396.

Mori, T., Wakashima, K., 1990. Successive iteration method in the evaluation of average fields in elastically inhomogeneous materials. In: Weng, G.J., Taya, M., Abe, H. (Eds.), Micromechanics and Inhomogeneity, Springer, New York, pp. 269–282.

Mura, T., 1987. Micromechanics of Defects in Solids. Martinus Nijhoff Publishers, Dordrecht.

Richard, T.G., 1975. The mechanical behavior of a solid microsphere filled composite. J. Comp. Mat. 9, 108–113.

Smith, J.C., 1976. Experimental values for the elastic constants of a particulate-filled glassy polymer. J. Res. NBS 80A, 45–49.