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ISSN: 0976-3376

ASIAN JOURNAL OF SCIENCE AND TECHNOLOGY

Asian Journal of Science and Technology
Vol. 08, Issue, 03, pp.4560-4564, March, 2017

RESEARCH ARTICLE

EQUIVALENT MODULUS OF COMPOSITES WITH RANDOMLY DISTRIBUTED NANOSIZED ELLIPSOIDAL INCLUSIONS

Ou Zhiying and *Ding Xiaoye

School of Science, Lanzhou University of Technology, Lanzhou 730050, P. R. China

ARTICLE INFO

Article History:
Received 17th December, 2016
Received in revised form
24th January, 2017
Accepted 14th February, 2017
Published online 31st March, 2017

Key words:

Composite Materials,
Equivalent Modulus,
Nanoscale, Ellipsoidal Inclusion.

ABSTRACT

The calculation of the equivalent modulus of the particle reinforced composite materials is an important part of composite materials mechanics, and there are two kinds of analytic methods for equivalent modulus. One is bound approaches and the other is direct estimations. This paper improved the methods mentioned above and obtained the local stress field of nano-rotating ellipsoidal inclusion based on the energy equivalence principle. The equivalent modulus of composite materials containing randomly distributed nano-ellipsoidal inclusions was also estimated.

INTRODUCTION

The determination of the effective elastic behavior for heterogeneous materials in terms of internal phases (inclusions and cavities) properties has been widely investigated during the past years. The calculation of the equivalent modulus of the particle reinforced composite materials is an important part of composite material mechanics, there are two kinds of analytic methods for equivalent modulus. One is bound approaches and the other is direct estimations. Both methods simplify the model and merely consider composite materials with random distribution of cylinder or ball. In this context, the self-consistent and Mori-Tanaka methods (Mori and Tanaka, 1973) which have been extensively used: they describe material in homogeneities as ellipsoidal inclusions isolated in a homogeneous medium applied to uniform remote load. Later, Bornert (Bornert, 1996) has obtained the equivalent modulus of composite materials containing ellipsoidal inclusions by using finite element method. In order to solve grid division and calculation increasing exponentially problem, Riccardi and Montheillet (Riccardi and Montheillet, 1999) have improved 3PM method proposed by Luo and Weng (Luo and Weng, 1987, 1989) to estimate the equivalent modulus of elliptical inclusion compound material.

****Corresponding author: Ding Xiaoye,***
School of Science, Lanzhou University of Technology, Lanzhou 730050, P. R. China.

It takes into account the complex interaction between matrix and inclusions by considering the representative inclusion as embedded in a finite matrix layer, which is itself embedded in the effective medium. Even so, they have neglected the influence of interface stress when the scale of ellipsoidal inclusion is nanometer grade. Huang et al. (Huang *et al.,* 1994, 1995) have proposed a generalized self-consistent method, to determine the in-plane effective moduli of a transversely isotropic material containing unidirectionally aligned cylindrical inclusions, the elliptical cross section of the latter being randomly oriented in the transverse plane. In this paper, we propose a method which avoids the latter difficulties, for a heterogeneous material containing single phase and randomly oriented ellipsoidal inclusions with the same aspect ratios. We improve the methods mentioned above and obtaine the local stress field of the nanosized ellipsoidal inclusion based on the energy equivalence principle. The equivalent moduli of composite materials containing randomly distributed nano-ellipsoidal inclusions are also estimated in this paper.

Energy equivalence equation

Composite materials are constitute of the matrix with Young's modulus E^{M} and Poisson's ratio ν^{M}, and $N-1$ kind of isotropic inclusions, which has its own shape (*s*=*a*/*b*, short half axis *a*, major half axis *b*), orientation, elastic modulus E^{I}, Poisson's ratio ν^{I} and volume percentage f_1. In general, composite materials is anisotropic on the macro materials, their equivalent moduli are expressed as the tensor $\bar{C}_{klmn}$. In order to get the equivalent moduli, we need to apply a force σ^0_{kl} on materials with volume V of as shown in figure 1.

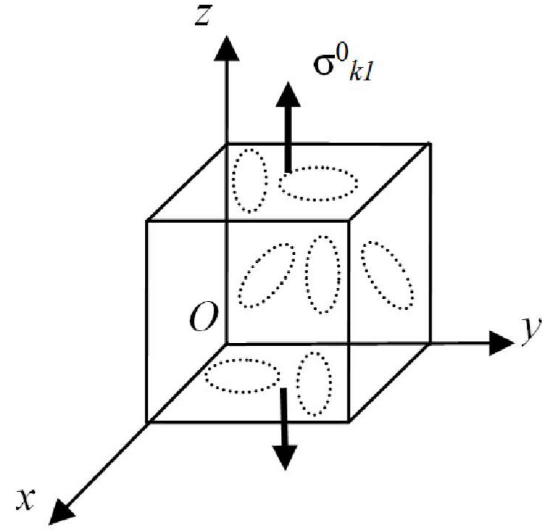

Fig.1. Composites with randomly distributed ellipsoidal inclusion

Considering the volume V of composite materials, their total strain U can be expressed by (Budiansky, 1965) as

$$U=\frac{1}{2}\int_V \sigma_{kl}\varepsilon_{kl}dV=\frac{1}{2}\left\{\frac{1+\upsilon^{\mathrm{M}}}{E^{\mathrm{M}}}\sigma^0_{kl}\sigma^0_{kl}-\frac{\upsilon^{\mathrm{M}}}{E^{\mathrm{M}}}\sigma^0_{kk}\sigma^0_{ll}+\right.$$

$$\left.+\sum_{\mathrm{I}=1}^{N-1}f_{\mathrm{I}}\left[\left(1-\frac{1+\upsilon^{\mathrm{M}}}{1+\upsilon^{\mathrm{I}}}\frac{E^{\mathrm{I}}}{E^{\mathrm{M}}}\right)\sigma^0_{kl}\varepsilon^{\mathrm{I}}_{kl}+\frac{\upsilon^{\mathrm{M}}-\upsilon^{\mathrm{I}}}{\left(1-2\upsilon^{\mathrm{I}}\right)\left(1+\upsilon^{\mathrm{I}}\right)}\frac{E^{\mathrm{I}}}{E^{\mathrm{M}}}\sigma^0_{kk}\varepsilon^{\mathrm{I}}_{ll}\right]\right\}V$$

$$=\frac{1}{2}\left(C^e_{klmn}\right)^{-1}\sigma^0_{kl}\sigma^0_{mn}V \quad \ldots\ldots (1)$$

Where (I, M) indicate inclusions and matrix respectively; (E,υ) represent Young's modulus and Poisson's ratio, f_{I} is the first I kind of volume percentage.

Here $\varepsilon^{\mathrm{I}}_{kl}=\frac{1}{V_{\mathrm{I}}}\int_{V_{\mathrm{I}}}\varepsilon_{kl}dV$ is the average strain in the I^{th} inclusion and $V_{\mathrm{I}}=f_{\mathrm{I}}V$.

The energy equation can be written in simple

$$\frac{1}{\mu^e}=\frac{1}{\mu^{\mathrm{M}}}+f_{\mathrm{I}}\left(1-\frac{\mu^{\mathrm{I}}}{\mu^{\mathrm{M}}}\right)\left\langle\varepsilon^{I(A)}_{ZZ}\right\rangle \quad \ldots\ldots (2)$$

$$\frac{1}{K^e}=\frac{1}{K^{\mathrm{M}}}+f_{\mathrm{I}}\left(1-\frac{K^{\mathrm{I}}}{K^{\mathrm{M}}}\right)\left\langle tr\left[\varepsilon^{I(H)}\right]\right\rangle \quad \ldots\ldots (3)$$

where $tr[\square]$ is the trace tensorial operator, the index I is associated with the inclusion phase, and (μ^e,K^e), $(\mu^{\mathrm{M}},K^{\mathrm{M}})$ and $(\mu^{\mathrm{I}},K^{\mathrm{I}})$ are the shear and bulk moduli of the effective medium, matrix and inclusion, respectively. The axisymmetric (A) and hydrostatic (H) remote loadings are defined, in the macroscopic axes $(OXYZ)$ (Fig. 2), by

$$\text{(A)}: \begin{cases}\sigma^0_{XX}=\sigma^0_{YY}=-\sigma^0, \quad \sigma^0_{ZZ}=2\sigma^0\\ \sigma^0_{YZ}=\sigma^0_{XZ}=\sigma^0_{XY}=0\end{cases} \quad \ldots\ldots (4)$$

$$\text{(H)}: \begin{cases}\sigma^0_{XX}=\sigma^0_{YY}=\sigma^0_{ZZ}=\sigma^0\\ \sigma^0_{YZ}=\sigma^0_{XZ}=\sigma^0_{XY}=0\end{cases} \quad \ldots\ldots (5)$$

The average of $tr\left[\varepsilon^{I(H)}\right]$ over the inclusion orientations is trivially calculated, since both the trace operator and the hydrostatic loading (H) are independent on (θ,φ).

$$\left\langle tr\left[\varepsilon^{I(\mathrm{H})}\right]\right\rangle=\frac{1}{2\pi}\int_0^{\pi/2}\sin\theta d\theta\int_0^{2\pi}tr\left[\varepsilon^{I(\mathrm{H})}\right]d\varphi$$

$$=\varepsilon^{I(zz)}_{zz}+2\varepsilon^{I(zz)}_{xx}+\varepsilon^{I(xx,yy)}_{zz}+2\varepsilon^{I(xx,yy)}_{xx} \quad \ldots\ldots (6)$$

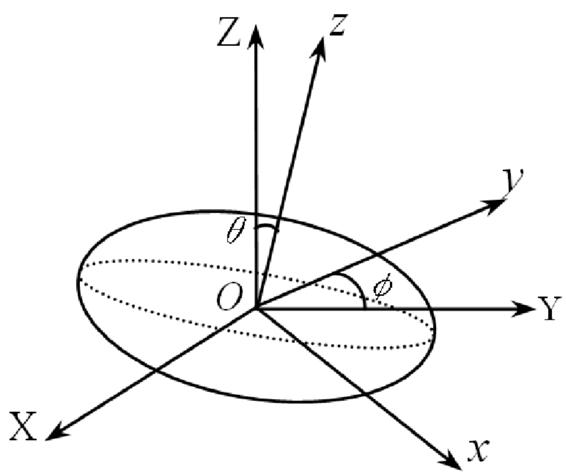

Fig. 2. Oblate spheroidal inclusion oriented at arbitrary angles (θ,φ)

To integrate the volume average strain $\left\langle\varepsilon^{I(\mathrm{A})}_{ZZ}\right\rangle$ over the inclusion orientations, we have

$$\varepsilon^{I(\mathrm{A})}_{ZZ}(\theta,\varphi)=\cos^2\theta\varepsilon^{I(\mathrm{A})}_{zz}(\varphi)-\sin 2\theta\varepsilon^{I(\mathrm{A})}_{xz}(\varphi)+\sin^2\theta\varepsilon^{I(\mathrm{A})}_{xx}(\varphi) \quad \ldots\ldots (7)$$

Then, the dependence of the volume average strain on the inclusion orientation is obtained through the decomposition of axisymmetric load (A) in the inclusion coordinate. Taking the symmetries of the problem into account, the final result is given by

$$\left\langle\varepsilon^{I(\mathrm{A})}_{ZZ}(\theta,\varphi)\right\rangle=\frac{1}{2\pi}\int_0^{\pi/2}\sin\theta d\theta\int_0^{2\pi}\varepsilon^{I(\mathrm{A})}_{ZZ}(\theta,\varphi)d\varphi$$

$$=\frac{4}{15}\left(\varepsilon^{I(zz)}_{zz}-\varepsilon^{I(zz)}_{xx}\right)-\frac{2}{15}\left(\varepsilon^{I(xx,yy)}_{zz}-\varepsilon^{I(xx,yy)}_{xx}\right)+\frac{4}{5}\varepsilon^{I(xx,-yy)}_{xx}+\frac{4}{5}\varepsilon^{I(xz)}_{xz} \quad \ldots\ldots (8)$$

Using (2), (3), (6) and (8), the energy equivalence equation is then given in the inclusion coordinate ($Oxyz$) by

$$\frac{1}{\mu^e}=\frac{1}{\mu^{\mathrm{M}}}+f_{\mathrm{I}}\left(1-\frac{\mu^{\mathrm{I}}}{\mu^{\mathrm{M}}}\right)$$

$$\left[\frac{4}{15}\left(\varepsilon^{I(zz)}_{zz}-\varepsilon^{I(zz)}_{xx}\right)-\frac{2}{15}\left(\varepsilon^{I(xx,yy)}_{zz}-\varepsilon^{I(xx,yy)}_{xx}\right)+\frac{4}{5}\varepsilon^{I(xx,-yy)}_{xx}+\frac{4}{5}\varepsilon^{I(xz)}_{xz}\right] \quad \ldots\ldots (9)$$

$$\frac{1}{K^e}=\frac{1}{K^{\mathrm{M}}}+f_1\left(1-\frac{K^{\mathrm{I}}}{K^{\mathrm{M}}}\right)\left[\varepsilon_{zz}^{I(zz)}+2\varepsilon_{xx}^{I(zz)}+\varepsilon_{zz}^{I(xx,yy)}+2\varepsilon_{xx}^{I(xx,yy)}\right] \quad \text{………. (10)}$$

As noted by Huang *et al*. (Huang *et al.,* 1995), the energy equivalence equations (9), (10) and (1) are exact. An approximate description of a single inclusion in the heterogeneous material is then adopted and the volume average strains are evaluated by solving the associated localization problems. Here, we choose to adapt the classical three phase model to materials containing randomly oriented spheroidal inclusions.

Computation of the inclusion volume average strains

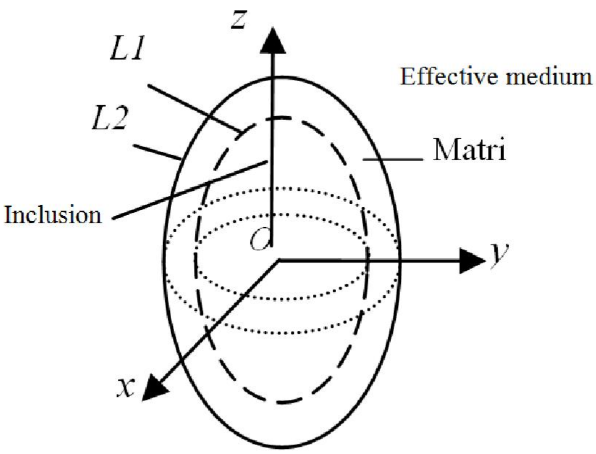

Fig. 3. Representative volume element of the material consisting of an ellipsoidal duplex inclusion

Figure 3 shows the representative volume element of the three-phase ellipsoidal inclusion. Ellipsoidal inclusion locates within L1, the part between L1 and L2 is the matrix, and the outermost part is equivalent medium. L1 and L2 are confocal rotational ellipsoids. The volume ratio of ellipsoid L1 and L2 is the percent of the inclusions f_{I}. According to the previous analysis, the solution of balance equation expressed in the displacement component can be represented in four harmonic potential functions, in order to be more clearly, we repeat by (Ou *et al.,* 2009) as follows

$$2\mu\left[u_\alpha,u_\beta,u_\gamma\right]=grad\left(\varphi_0+c\overline{pq}\cos\gamma\varphi_1+c\overline{pq}\sin\gamma\varphi_2+cpq\varphi_3\right)$$

$$-4(1-\upsilon)[\varphi_1,\varphi_2,\varphi_3] \quad \text{……………………………………… (11)}$$

In the ellipsoidal coordinate system, the harmonic potential functions are expanded in series of Legendre functions.

$$\left(\xi_n P_n^m(q)+\eta_n Q_n^m(q)\right)P_n^m(p)\left(\cos m\gamma \ or \sin m\gamma\right) \quad \text{……………….. (12)}$$

Where m is an integer. P_n^m are Legendre functions of the first kind, Q_n^m are Legendre functions of the second kind. P_n^m and Q_n^m can be expanded by (Cooke, 1956) as follows

$$P_n(q)=\frac{1}{2^n n!}\frac{d^n}{dq^n}(q^2-1)^n \quad \text{……………………………… (13)}$$

$$Q_n(q)=\frac{1}{2}P_n(q)\log\left(\frac{q+1}{q-1}\right)-W_{n-1}(q) \quad \text{……………………….. (14)}$$

$$W_{n-1}(q)=\sum_{j=1}^{n}\frac{1}{j}P_{j-1}(q)P_{n-j}(q) \quad \text{…………………………… (15)}$$

For the different loading, the specific displacement potential functions of each part are different, e.g.

(zz): $\sigma_{xx}^0=\sigma_{yy}^0=0,\quad \sigma_{zz}^0=\sigma^0,\quad \sigma_{yz}^0=\sigma_{xz}^0=\sigma_{xy}^0=0$

In the case of the loading (zz), the analytic displacement potential functions are:

In the inclusion,

$$\varphi_0^{\mathrm{I}}=\sigma^0\sum_{n=0}^{\infty}A_n^{\mathrm{I}}P_n(q)P_n(p) \quad \text{………………………………….. (16)}$$

$$\varphi_1^{\mathrm{I}}=\varphi_2^{\mathrm{I}}=0 \quad \text{……………………………………. (17)}$$

$$\varphi_3^{\mathrm{I}}=\sigma^0\sum_{n=0}^{\infty}B_n^{\mathrm{I}}P_n(q)P_n(p) \quad \text{…………………………………… (18)}$$

Within the matrix,

$$\varphi_0^{\mathrm{M}}=\sigma^0\sum_{n=0}^{\infty}\left[A_n^{\mathrm{M}}Q_n(q)+A_n^{\mathrm{M}}P_n(q)\right]P_n(p) \quad \text{…………………….. (19)}$$

$$\varphi_1^{\mathrm{M}}=\varphi_2^{\mathrm{M}}=0 \quad \text{…………………...…………… (20)}$$

$$\varphi_3^{\mathrm{M}}=\sigma^0\sum_{n=0}^{\infty}\left[C_n^{\mathrm{M}}Q_n(q)+D_n^{\mathrm{M}}P_n(q)\right]P_n(p) \quad \text{…………………..…. (21)}$$

Within the equivalent medium,

$$\varphi_0^{e}=\sigma^0\sum_{n=0}^{\infty}E_n^{e}Q_n(q)P_n(p)+\varphi_0^0 \quad \text{…………………………. (22)}$$

$$\varphi_1^{e}=\varphi_2^{e}=0 \quad \text{………………………….. (23)}$$

$$\varphi_3^{e}=\sigma^0\sum_{n=0}^{\infty}F_n^{e}Q_n(q)P_n(p)+\varphi_3^0 \quad \text{………………………….. (24)}$$

Substituting the displacement potential functions of inclusions, matrix and equivalent medium under different loading into the equation (11), and in the light of constitute laws and the geometric equation, the displacement and stress with undetermined coefficients are obtained. Then by substitution of those into the following boundary conditions (25) to (29), the undetermined coefficients in the displacement potential function are obtained. And displacement field under the different loading are obtained. In the prolate spheroidal system, the boundary conditions equation on the L1 and L2 interface read.

In the interface L1,

$$u_\alpha^{\mathrm{M}}-u_\alpha^{\mathrm{I}}=0\,,\ u_\beta^{\mathrm{M}}-u_\beta^{\mathrm{I}}=0\,,\ u_\gamma^{\mathrm{M}}-u_\gamma^{\mathrm{I}}=0\,. \quad \text{………………….. (25)}$$

$$\sigma_{\alpha\alpha}^{(\mathrm{M})}-\sigma_{\alpha\alpha}^{(\mathrm{I})}=\left\{K_1\mu^{\mathrm{M}}+\sigma_{11}^{\mathrm{M}}\left[K_2\frac{(1-\upsilon)}{2(1+\upsilon)}+K_3\frac{1}{(1+\upsilon)}-\frac{K_1}{2}\right]+\sigma_{22}^{\mathrm{M}}\right.$$

$$\left[K_2\frac{(1-\upsilon)}{2(1+\upsilon)}-K_3\frac{\upsilon}{(1+\upsilon)}+\frac{K_1}{2}\right]-\sigma_{33}^{M}\left(K_2+K_3\right)\frac{\upsilon}{(1+\upsilon)}\Bigg\}b\kappa_{11}$$

$$+\Bigg\{K_1\mu^{M}+\sigma_{11}^{M}\left[K_2\frac{(1-\upsilon)}{2(1+\upsilon)}-K_3\frac{\upsilon}{(1+\upsilon)}+\frac{K_1}{2}\right]+\sigma_{22}^{M}$$

$$\left[K_2\frac{(1-\upsilon)}{2(1+\upsilon)}+K_3\frac{1}{(1+\upsilon)}-\frac{K_1}{2}\right]-\sigma_{33}^{M}\left(K_2+K_3\right)\frac{\upsilon}{(1+\upsilon)}\Bigg\}b\kappa_{22}\quad\ldots(26)$$

$$\sigma_{\alpha\beta}^{(M)}-\sigma_{\alpha\beta}^{(I)}-cq\overline{p}\Bigg\{\left[\left[\frac{(1-\upsilon)K_2}{2(1+\upsilon)}+\frac{K_3}{(1+\upsilon)}-\frac{K_1}{2}\right]\frac{\partial\sigma_{11}^{M}}{\partial p}\right.$$

$$\left.+\left[\frac{(1-\upsilon)K_2}{2(1+\upsilon)}-\frac{K_3\upsilon}{(1+\upsilon)}+\frac{K_1}{2}\right]\frac{\partial\sigma_{22}^{M}}{\partial p}-\left(K_2+K_3\right)\frac{\upsilon}{(1+\upsilon)}\frac{\partial\sigma_{33}^{M}}{\partial p}\right\}$$

$$+2cq\left(K_3-K_1\right)\frac{\partial\tau_{12}^{M}}{\partial\gamma}=0\qquad\ldots\ldots(27)$$

$$\sigma_{\alpha\gamma}^{(M)}-\sigma_{\alpha\gamma}^{(I)}-2cq\overline{p}\left(K_3-K_1\right)\frac{\partial\tau_{12}^{M}}{\partial p}+\left[K_2\frac{(1-\upsilon)}{2(1+\upsilon)}-K_3\frac{\upsilon}{(1+\upsilon)}+\frac{K_1}{2}\right]$$

$$\frac{\partial\sigma_{11}^{M}}{\partial\gamma}+\left[K_2\frac{(1-\upsilon)}{2(1+\upsilon)}+K_3\frac{1}{(1+\upsilon)}-\frac{K_1}{2}\right]\frac{\partial\sigma_{22}^{M}}{\partial\gamma}-cq\left(K_2+K_3\right)$$

$$\frac{\upsilon}{(1+\upsilon)}\frac{\partial\sigma_{33}^{M}}{\partial\gamma}=0\qquad\ldots\ldots(28)$$

Where $K_1=\dfrac{\tau_0}{b\mu^{M}}$, $K_2=\dfrac{\lambda^{s}}{b\mu^{M}}$, $K_3=\dfrac{\mu^{s}}{b\mu^{M}}$.

In the interface L2,

$$u_{\alpha}^{M}-u_{\alpha}^{e}=0,\; u_{\beta}^{M}-u_{\beta}^{e}=0,\; u_{\gamma}^{M}-u_{\gamma}^{e}=0\qquad\ldots\ldots(29)$$

$$\sigma_{\alpha\alpha}^{M}-\sigma_{\alpha\alpha}^{e}=0,\; \sigma_{\alpha\beta}^{M}-\sigma_{\alpha\beta}^{e}=0,\; \sigma_{\alpha\gamma}^{M}-\alpha_{\alpha\gamma}^{e}=0\qquad\ldots\ldots(30)$$

Finally, substituting the strains of the inclusion into equations (9) and (10), one obtains the equivalent moduli.

RESULTS AND DISCUSSION

In what follows, the numerical results of equivalent modulus of composite with the nano-ellipsoidal inclusions are given. In numerical calculations, let $s=\dfrac{a}{b}$ = 1/2 for ellipsoidal inclusion and s = 1 for spherical inclusion, and the different volume percentages (f_{I} =0.1, 0.3, 0.5), and assume $\upsilon^{I}=\upsilon^{M}=0.3$ and $\Gamma=\mu^{\mathrm{I}}/\mu^{\mathrm{M}}$. For simplicity, the effect of surface elastic constants limited to $\lambda^{s}/\left(b\mu^{M}\right)$ on the effective moduli is studied. Figure 4 and figure 5 show that the equivalent shear modulus and bulk modulus of the composites vary with the surface elastic constant under the different volume percentages of the soft and hard inclusions. s=0.5 indicates the ratio of the short half axis to the major half axis of the ellipsoid.

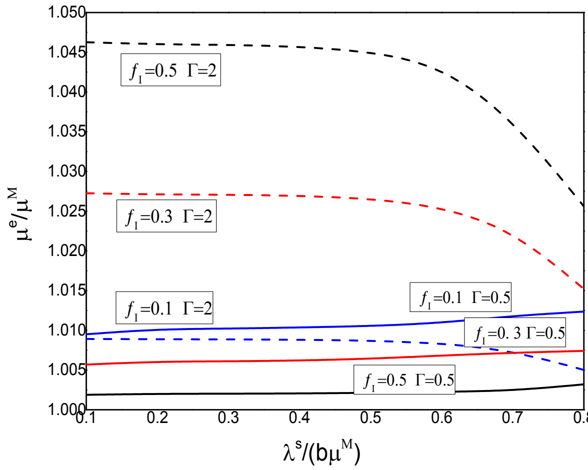

Fig. 4. Relationship between equivalent shear modulus and surface elastic constant

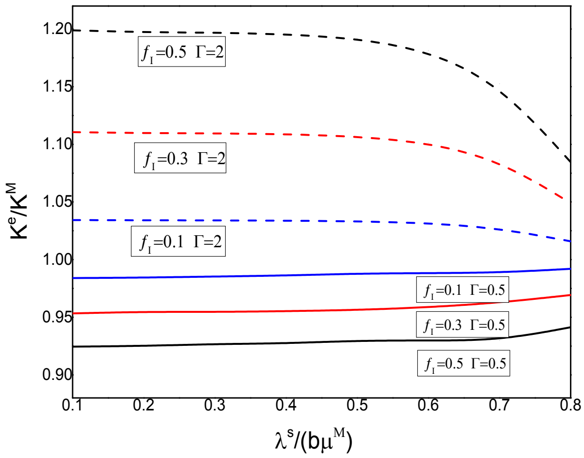

Fig. 5. Relationship between equivalent bulk modulus and surface elastic constant

It can be seen that the relationship between equivalent modulus and $\lambda^{s}/\left(b\mu^{M}\right)$ is a nonlinear. The effective modulus are decreasing with the $\lambda^{s}/\left(b\mu^{M}\right)$ for hard inclusions, and the change is violent when the $\lambda^{s}/\left(b\mu^{M}\right)$<0.6. The equivalent modulus are gradually increasing with the $\lambda^{s}/\left(b\mu^{M}\right)$ for soft inclusions, and the change is less evident when the $\lambda^{s}/\left(b\mu^{M}\right)$ <0.6. Simultaneously, the higher is volume percent of hard inclusions, the higher is the equivalent moduli. For soft inclusions, the results are inverse. Further analysis shows that, if a material λ^{s}/μ^{M} is fixed, these equivalent modulus are inversely proportional to the quantity b representing the size of the inclusions. It is obvious that the effect of size needs to be considered under the nano-mechanics. The relationship between equivalent moduli and the surface elastic constant under the different volume percentages of soft inclusions and hard inclusions are shown in figure 6 and figure 7, respectively. s=1 indicates that the spheroidal inclusions embedded in the composite. The results show that the equivalent bulk modulus and the equivalent shear modulus are numerical different from those embedded in nano-ellipsoidal inclusions, and the variable trend with the surface elastic constant is roughly the same.

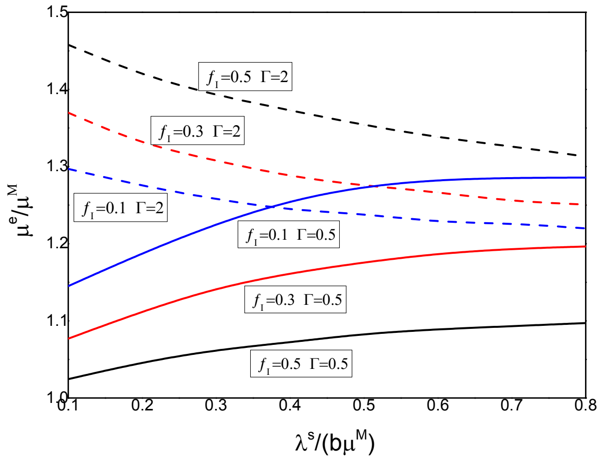

Fig. 6. Relationship between equivalent shear modulus and surface elastic constant

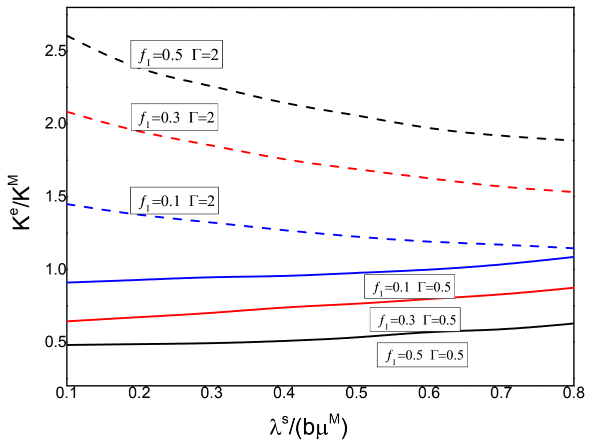

Fig.7. Relationship between equivalent bulk modulus and surface elastic constant

Conclusions

Under the consideration of interface effect, the paper is the successful application of three-phase ellipsoid model to estimate the equivalent moduli of composites embedded in the random distribution of rotating ellipsoid inclusions. The effective modulus depend on material intrinsic length (λ^s/μ^M) and characteristic size of ellipsoid (*b, s*).

Acknowledgements

This work was supported in part by the National Natural Science Foundation (Grant No. 1106004 and 11362009).

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