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Prediction of the dynamic effective properties of particle-reinforced composite materials

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Abstract: The prediction behaviors of some coherent plane wave equations for the effective velocities and attenuations of the coherent plane waves propagating through a composite material and for the effective elastic moduli of the composites are studied. The numerical results obtained by Waterman & Truell's, Twersky's and Gubernatis's equations for Glass-Epoxy composites with various volume fractions are compared. It is found that the predictions by both Twersky's and Gubernatis's equations underestimate the effective velocities and the effective elastic moduli when compare with the predictions by Waterman & Truell's equation. Furthermore, the deviations are more evident for the shear wave than that for the longitudinal wave. But these deviations decrease gradually with the increase of the frequency and increase gradually with the increase of the volume fraction.

Key words: coherent plane waves; prediction behavior; effective velocity; effective attenuation

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1 Introduction

When an acoustic or elastic wave propagates through a composite material with randomly distributed reinforced particles or fibers, the multiple scattering amongst these scatterers arises due to the spatial inhomogeneity. In general, the total wave field in a composite medium can be regarded as the sum of the mean wave field and the fluctuating wave field. The mean wave field (coherent wave field) can be considered as the wave field propagating in the homogeneous medium having the effective properties of the composite materials and the fluctuating wave field (incoherent wave field) can be considered as the wave field due to the randomly spatial variations of material properties from those of the effective medium. The propagation constants of the mean or coherent plane wave and the dynamic effective elastic moduli of the homogeneous effective medium are of importants and have attracted considerably attentions [1-14]. In these studies the main approaches to simplify the interaction amongst the scatterers are the effective exciting field approach [1-4] and the effective medium approach [5,9,10,12]. For a relatively high volume fraction, the effective medium approach and the effective field approach with the pair-correlation function involved are usually considered. In general, no explicit expressions of the effective properties of composite materials can be obtained except in the Rayleigh limits. However, for a relatively low volume fraction, the correlation in the positions of the particles or fibers can be ignored, and some explicit expressions of the effective properties are thus obtained. The prediction behaviors of these expressions should be investigated by comparison. Regretfully, such a work is rare in the literatures. It is our purpose to study on the prediction behaviors of these explicit equations by comparison of their numerical results.

2 Far-field scattering amplitudes

In the case of an incident scalar wave

$$\varphi^{i}=e^{i(kz-\omega t)} \tag{1}$$

The scattered wave in the far-field $\boldsymbol{r}$ scattered by a single scatterer which is located at $\boldsymbol{r}'$ can be expressed asymptotically as

$$\varphi^{s}=f(\theta,\phi)\frac{e^{ik(|\boldsymbol{r}-\boldsymbol{r}'|)}}{|\boldsymbol{r}-\boldsymbol{r}'|}e^{-i\omega t} \tag{2}$$

where $f(\theta,\phi)$ is called the azimuth-dependent far-field scattered amplitude and (θ,ϕ) are the azimuth angles.

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In the case of an incident vector wave

$$\boldsymbol{u}^{\mathrm{i}} = \boldsymbol{a} e^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)} \tag{3}$$

where $\boldsymbol{a}$ is the unit polarization vectors of an incident vector wave, $\boldsymbol{k}$ is the wavenumber vector. The scattered wave in the far-field scattered by the same scatterer which is located at $\boldsymbol{r}'$ can be expressed asymptotically as

$$\boldsymbol{u}^{\mathrm{s}} = \boldsymbol{F}(\theta,\phi)\frac{\mathrm{e}^{\mathrm{i}|\boldsymbol{k}||\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|}\mathrm{e}^{-\mathrm{i}\omega t} \tag{4}$$

where $\boldsymbol{F}(\theta,\phi)$ is called the azimuth-dependent far-field scattered amplitude vector. The projection of this vector in the polarization vector, $f(\theta,\phi)=\boldsymbol{F}(\theta,\phi)\cdot\boldsymbol{a}$, is defined as the far-field scattered amplitude.

In the case of the incident elastic waves which is considered in the present work, *i.e.*

$$\boldsymbol{u}^{\mathrm{i}} = \boldsymbol{a} e^{\mathrm{i}(k_{\mathrm{p}0}z-\omega t)} + \boldsymbol{b} e^{\mathrm{i}(k_{\mathrm{s}0}z-\omega t)} \tag{5}$$

where $\boldsymbol{a}$ and $\boldsymbol{b}$ are the polarization vectors of the incident P and S waves, respectively; $k_{\mathrm{p}0}$ and $k_{\mathrm{s}0}$ are the wavenumbers of the incident P and S waves. In the far-field, the wave scattered by a single scatterer which is located at $\boldsymbol{r}'$ can be expressed asymptotically as

$$\boldsymbol{u}^{\mathrm{s}}(\boldsymbol{r}\,|\,\boldsymbol{r}') = \frac{\boldsymbol{F}_{\mathrm{p}}(k_{\mathrm{p}0},k_{\mathrm{s}0},\theta,\phi)}{|\boldsymbol{r}-\boldsymbol{r}'|}\mathrm{e}^{\mathrm{i}k_{\mathrm{p}0}|\boldsymbol{r}-\boldsymbol{r}'|} + \frac{\boldsymbol{F}_{\mathrm{s}}(k_{\mathrm{p}0},k_{\mathrm{s}0},\theta,\phi)}{|\boldsymbol{r}-\boldsymbol{r}'|}\mathrm{e}^{\mathrm{i}k_{\mathrm{s}0}|\boldsymbol{r}-\boldsymbol{r}'|} \tag{6}$$

The corresponding far-field scattered amplitudes of the P and S waves are

$$\begin{cases} f_{\mathrm{p}}(\theta,\phi) = \boldsymbol{F}_{\mathrm{p}}(k_{\mathrm{p}0},k_{\mathrm{s}0},\theta,\phi)\cdot\boldsymbol{a} \\ f_{\mathrm{s}}(\theta,\phi) = \boldsymbol{F}_{\mathrm{s}}(k_{\mathrm{p}0},k_{\mathrm{s}0},\theta,\phi)\cdot\boldsymbol{b} \end{cases} \tag{7}$$

In general, the scattered wave field can be related with the exciting wave field by

$$\boldsymbol{u}^{\mathrm{s}} = \boldsymbol{T}^{\mathrm{s}}\boldsymbol{u}^{\mathrm{i}} \tag{8}$$

where $\boldsymbol{T}^{\mathrm{s}}$ is the scattering operator which is dependent upon the properties and shape of the scatterer as well as the properties of the host medium where the scatterer is embedded. For a spherical scatterer, by employing the eighfunction expansion technique and the asymptotic expression of the radial function $h_n^{(1)}(kr)$, *i.e.*

$$h_n^{(1)}(kr) \sim \frac{1}{kr}\mathrm{e}^{\mathrm{i}[kr-\frac{1}{2}(n+1)\pi]} + o(\frac{1}{r}),\ \text{when}\ r\to\infty \tag{9}$$

The displacement of scattered waves in the far-field can be expressed asymptotically

$$u_r = \frac{F_r(\theta,\phi)}{r}\mathrm{e}^{\mathrm{i}k_{\mathrm{p}0}r} + o(\frac{1}{r}) = \frac{1}{r}\mathrm{e}^{\mathrm{i}k_{\mathrm{p}0}r}\sum_{n=0}^{\infty}\sum_{m=0}^{\pm n}\mathrm{i}A_{mn}^{\mathrm{s}}\mathrm{e}^{-\mathrm{i}\frac{1}{2}(n+1)\pi}P_n^m(\cos\theta)\mathrm{e}^{im\phi} + o(\frac{1}{r}) \tag{10a}$$

$$\begin{aligned} u_\theta &= \frac{F_\theta(\theta,\phi)}{r}\mathrm{e}^{\mathrm{i}k_{\mathrm{s}0}r} + o(\frac{1}{r}) \\ &= \frac{1}{r}\mathrm{e}^{\mathrm{i}k_{\mathrm{s}0}r}\sum_{n=0}^{\infty}\sum_{m=0}^{\pm n}\mathrm{i}\mathrm{e}^{-\mathrm{i}\frac{1}{2}(n+1)\pi}[B_{mn}^{\mathrm{s}}\frac{m}{k_{\mathrm{s}0}\sin\theta}P_n^m(\cos\theta) + C_{mn}^{\mathrm{s}}\frac{\mathrm{d}}{\mathrm{d}\theta}P_n^m(\cos\theta)]\mathrm{e}^{im\phi} + o(\frac{1}{r}) \end{aligned} \tag{10b}$$

$$u_\varphi = \frac{F_\varphi(\theta,\phi)}{r}\mathrm{e}^{\mathrm{i}k_{\mathrm{s}0}r} + o(\frac{1}{r}) = -\frac{1}{r}\mathrm{e}^{\mathrm{i}k_{\mathrm{s}0}r}\sum_{n=0}^{\infty}\sum_{m=0}^{\pm n}[\frac{B_{mn}^{\mathrm{s}}}{k_{\mathrm{s}0}}\frac{\mathrm{d}}{\mathrm{d}\theta}P_n^m(\cos\theta) + \frac{m}{\sin\theta}C_{mn}^{\mathrm{s}}P_n^m(\cos\theta)]\mathrm{e}^{-\mathrm{i}\frac{1}{2}(n+1)\pi}e^{im\phi} + o(\frac{1}{r}) \tag{10c}$$

where the extension coefficients A_{mn}^{s}, B_{mn}^{s} and C_{mn}^{s} are determined by the continuous conditions of the displacements and the tractions at the interface between the scatterer and the host medium, $P_n^m(\cos\theta)$ is the associated Legendre function. The far-field scattered amplitude vectors for the scattered longitudinal and shear waves can be written as $\boldsymbol{F}_{\mathrm{p}} = F_r(\theta,\phi)\boldsymbol{e}_r$ and $\boldsymbol{F}_{\mathrm{s}} = F_\theta(\theta,\phi)\boldsymbol{e}_\theta + F_\varphi(\theta,\phi)\boldsymbol{e}_\varphi$ ($\boldsymbol{e}_r$, $\boldsymbol{e}_\theta$ and $\boldsymbol{e}_\varphi$ is unit polar coordinate vectors), respectively. The far-field scattered amplitudes at two specific azimuthal angles, $\theta=0$ and $\theta=\pi$, are called the forward and the backward scattering amplitudes, respectively, and will play important roles in predicting the effective properties of a composite material.

$$\begin{cases} F_r(0,\phi) = \sum_{n=0}^{\infty}(-\mathrm{i})^n A_{0n}^{\mathrm{s}} \\ F_\theta(0,\phi) = \sum_{n=1}^{\infty}\frac{(-\mathrm{i})^n}{2}[\frac{n(n+1)}{k_{\mathrm{s}0}}B_{1n}^{\mathrm{s}}\mathrm{e}^{\mathrm{i}\phi} + \frac{1}{k_{\mathrm{s}0}}B_{-1n}^{\mathrm{s}}\mathrm{e}^{-\mathrm{i}\phi}] \\ F_\varphi(0,\phi) = \sum_{n=1}^{\infty}\frac{\mathrm{i}(-\mathrm{i})^n}{2}[n(n+1)C_{1n}^{\mathrm{s}}\mathrm{e}^{\mathrm{i}\phi} + C_{-1n}^{\mathrm{s}}\mathrm{e}^{-\mathrm{i}\phi}] \end{cases} \tag{11}$$

$$\begin{cases} F_r(\pi,\phi) = \sum_{n=0}^{\infty}\mathrm{i}^n A_{0n}^{\mathrm{s}} \\ F_\theta(\pi,\phi) = \sum_{n=1}^{\infty}\frac{-\mathrm{i}^n}{2}[\frac{n(n+1)}{k_{\mathrm{s}0}}B_{1n}^{\mathrm{s}}\mathrm{e}^{\mathrm{i}\phi} + \frac{1}{k_{\mathrm{s}0}}B_{-1n}^{\mathrm{s}}\mathrm{e}^{-\mathrm{i}\phi}] \\ F_\varphi(\pi,\phi) = \sum_{n=1}^{\infty}\frac{-\mathrm{i}^{n+1}}{2}[n(n+1)C_{1n}^{\mathrm{s}}\mathrm{e}^{\mathrm{i}\phi} + C_{-1n}^{\mathrm{s}}\mathrm{e}^{-\mathrm{i}\phi}] \end{cases} \tag{12}$$

3 Coherent plane wave equations

In a composite material with randomly distributed inclusions whose positions are denoted by $(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_N)$, the total field at any point $\boldsymbol{r}$ outside all scatterers can be given in the multiple scattering form

$$\boldsymbol{u}(\boldsymbol{r};\boldsymbol{r}_1,\boldsymbol{r}_2,\cdots,\boldsymbol{r}_N)=\boldsymbol{u}^{\mathrm{i}}(\boldsymbol{r})+\sum_{k=1}^{N}\boldsymbol{T}^{\mathrm{s}}(\boldsymbol{r}_k)\boldsymbol{u}^{\mathrm{i}}(\boldsymbol{r})+\sum_{m=1}^{N}\boldsymbol{T}^{\mathrm{s}}(\boldsymbol{r}_m)\sum_{k=1,k\neq m}^{N}\boldsymbol{T}^{\mathrm{s}}(\boldsymbol{r}_k)\boldsymbol{u}^{\mathrm{i}}(\boldsymbol{r})+\cdots \tag{13}$$

where the single summation denotes the primary scattered terms, the double summation denotes the secondary scattered terms and so on. The primary scattering is due to the incident waves alone, and the second scattering represents the rescattering of the primary scattered waves, *etc*. The multiple scattering process takes into account the interaction among the distributed inclusions accurately. However, it is difficulty to deal with in order to predict the effective properties of such a composite material. Hence the effective exciting field approximation is usually used to describe approximately the interaction among the distributed inclusions. In this approximation it is assumed that each inclusion is excited by an effective exciting field $\boldsymbol{u}^{\mathrm{e}}$. Then equation (13) can be approximately replaced by

$$\boldsymbol{u}(\boldsymbol{r};\boldsymbol{r}_1,\boldsymbol{r}_2,\cdots,\boldsymbol{r}_N)=\boldsymbol{u}^{\mathrm{i}}(\boldsymbol{r})+\sum_{k=1}^{N}\boldsymbol{T}^{\mathrm{s}}(\boldsymbol{r}_k)\boldsymbol{u}^{\mathrm{e}}(\boldsymbol{r}\mid\boldsymbol{r}_k;\boldsymbol{r}_1,\cdots'\cdots,\boldsymbol{r}_N) \tag{14}$$

where the first coordinate $\boldsymbol{r}$ indicates the field point of evaluation, and the $(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_N)$ indicates the dependence of the random function $\boldsymbol{u}$ on the specific configuration chosen. Symbol "'" means the absence of one variable. After performing the configurational average over equation (14), it follows

$$\langle\boldsymbol{u}(\boldsymbol{r};\boldsymbol{r}_1,\cdots,\boldsymbol{r}_N)\rangle=\boldsymbol{u}^{\mathrm{i}}(\boldsymbol{r})+\int n(\boldsymbol{r}_k)\boldsymbol{T}^{\mathrm{s}}(\boldsymbol{r}_k)\langle\boldsymbol{u}^{\mathrm{e}}(\boldsymbol{r}\mid\boldsymbol{r}_k;\boldsymbol{r}_1,\cdots'\cdots,\boldsymbol{r}_N)\rangle\mathrm{d}V_k \tag{15}$$

The quantity $\langle\boldsymbol{u}^{\mathrm{e}}(\boldsymbol{r}\mid\boldsymbol{r}_k;\boldsymbol{r}_1,\cdots'\cdots,\boldsymbol{r}_N)\rangle$ represents the exciting field acting on the k-th scatterer averaged over all possible configurations of the other scatterers. Therefore it is, in fact, the counterpart of the averaged total field with one inclusion absent. The deviation between the averaged total field with N inclusions involved, $\langle\boldsymbol{u}(\boldsymbol{r};\boldsymbol{r}_1,\cdots,\boldsymbol{r}_N)\rangle$, and the ones with one less inclusion involved, $\langle\boldsymbol{u}^{\mathrm{e}}(\boldsymbol{r}\mid\boldsymbol{r}_k;\boldsymbol{r}_1,\cdots'\cdots,\boldsymbol{r}_N)\rangle$, would become unnoticed as the number of inclusions are very large. Hence, we may make the self-consistent approximation

$$\langle\boldsymbol{u}_k^{\mathrm{e}}(\boldsymbol{r}\mid\boldsymbol{r}_k;\boldsymbol{r}_1,\cdots'\cdots,\boldsymbol{r}_N)\rangle\approx\langle\boldsymbol{u}(\boldsymbol{r};\boldsymbol{r}_1,\cdots,\boldsymbol{r}_N)\rangle \tag{16}$$

This approximation was proposed first by Foldy [1] and leads to the coherent plane scalar wave equation

$$(\frac{k_*}{k_0})^2=1+\frac{4\pi n}{k_0^2}f(k_0) \tag{17}$$

where k_* is the wavenumber of the coherent wave and k_0 is that of the incident wave, n is the number density of scatterers, $f(k_0)$ is the isotropic scattering amplitude scattered by a single inclusion embedded in a homogenous medium. It is noted that only the isotropic point scattering is considered in Foldy's work. This approximation was later modified by Lax [2] with introduction of a correction parameter c' and extended to the anisotropic scattering by replacing $f(k_0)$ with the forward scattering amplitude $f(k_0,0)$

$$(\frac{k_*}{k_0})^2=1+\frac{4\pi n}{k_0^2}c'f(k_0,0) \tag{18}$$

where the parameter c' is a measure of the ratio of the effective field $\langle\boldsymbol{u}^{\mathrm{e}}\rangle$ to the macroscopic average field $\langle\boldsymbol{u}\rangle$. Waterman & Truell provided a equation where the backward scattering amplitude $f(k_0,\pi)$ is also considered [3],

$$(\frac{k_*}{k_0})^2=[1+\frac{2\pi n}{k_0^2}f(k_0,0)]^2-[\frac{2\pi n}{k_0^2}f(k_0,\pi)]^2 \tag{19}$$

By only retaining the chain-scattering (neglecting the shuttle-scattering) in the multiple scattering processes, Twersky obtained [4,15]

$$k_*=k_0+\frac{2\pi n}{k_0}f(k_0,0) \tag{20}$$

Moreover, based on independent scattering approximation, Gubernatis [6] obtained

$$k_*^2=k_0^2+4\pi nf(k_*,0) \tag{21}$$

But often this equation is replaced by

$$k_*^2=k_0^2+4\pi nf(k_0,0) \tag{22}$$

For avoiding the burden of iterative process, by comparison of these equations, it is noted that Waterman & Truell's equation can reduce to Foldy's equation for the isotropic scattering where $f(k_0,0)=f(k_0,\pi)$, to Twersky's equation when the backward scattering amplitude is neglected, and to Gubernatis's equation when the second rank terms of the number density are neglected. Because the far-field scattering amplitudes are, in general, complex-valued and frequency-dependent, the effective wavenumbers of P and S waves, k_{p*} and k_{s*}, are thus complex-valued and frequency-dependent. The real part of the complex-valued wavenumber is related to the phase velocity and the imaginary part represents the attenuation of the coherent waves

$$\begin{cases} k_{p*}(\omega) = k_{p*}^{r}(\omega) + \mathrm{i}k_{p*}^{i}(\omega) = \omega/c_{p*} + \mathrm{i}\alpha_{p*} \\ k_{s*}(\omega) = k_{s*}^{r}(\omega) + \mathrm{i}k_{s*}^{i}(\omega) = \omega/c_{s*} + \mathrm{i}\alpha_{s*} \end{cases} \quad (23)$$

where c_{p*} and c_{s*} are the phase velocities, and α_{p*} and α_{s*} are the attenuations of P and S waves, respectively. Furthermore, the effective elastic moduli of the composite material can be obtained from the effective wavenumbers by

$$\begin{cases} G_*(\omega) = G_*^{r}(\omega) + \mathrm{i}G_*^{i}(\omega) = G_0 \dfrac{\rho_*}{\rho_0}(\dfrac{k_{s0}}{k_{s*}})^2 \\ K_*(\omega) = K_*^{r}(\omega) + \mathrm{i}K_*^{i}(\omega) = \\ \qquad (K_0 + \dfrac{4G_0}{3})\dfrac{\rho_*}{\rho_0}(\dfrac{k_{p0}}{k_{p*}})^2 - \dfrac{4}{3}G_0\dfrac{\rho_*}{\rho_0}(\dfrac{k_{s0}}{k_{s*}})^2 \end{cases} \quad (24)$$

where $G_*(\omega)$ and $K_*(\omega)$ are the frequency-dependent effective shear and bulk moduli of the composite material. G_0 and K_0 are the shear and bulk moduli of host medium. The effective density of the composite material, ρ_*, can be obtained approximately from the volume average,

$$\rho_* = (1-c)\rho_0 + c\rho_1 \quad (25)$$

where ρ_0 and ρ_1 are the densities of the host medium and the scatterer, respectively. c is the volume fraction of scatterers.

4 Comparison of the prediction behavior

The dynamic effective properties of a composite material, Glass-Epoxy, will be predicted in this section. The mechanical properties of the constituents are given in **table 1**.

In **figures 1**, **2**, and **3**, the predicted effective phase velocities, the effective attenuations and the effective elastic moduli from equations (19), (20) and (22), namely, Waterman & Truell's, Twersky's and Gubernatis's equations, are compared. It can be seen that Twersky's equation and Gubernatis's equation underestimate the effective phase velocities and the effective elastic moduli when compare with the predictions by Waterman & Truell's equations. However, the deviation decreases gradually with the increasing frequency. Although the predicted effective attenuations are also underestimated at any frequency by Twer-

Table 1 Constituent properties of composites: Glass-Epoxy [16]

Materials	K / GPa	G / GPa	ρ / (kg·m^{-3})	c_p / (m·s^{-1})	c_s / (m·s^{-1})
Epoxy	5.49	1.59	1180	2540	1160
Glass	34.56	26.14	2492	5280	3240

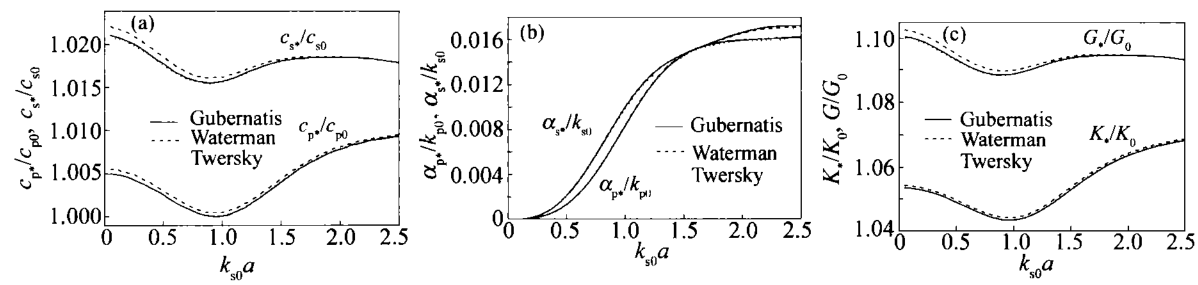

Figure 1 Effective phase velocities, effective attenuations and effective elastic moduli predicted by three coherent plane wave equations at the volume fraction c=0.05.

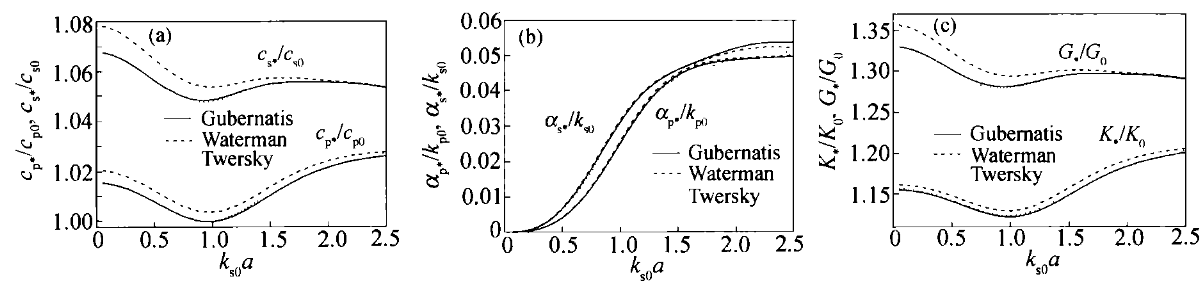

Figure 2 Effective phase velocities, effective attenuations and effective elastic moduli predicted by three coherent plane wave equations at the volume fraction c=0.15.

sky's equation when compare with the prediction obtained from Waterman &Truell's equation, but are underestimated at a relatively low frequency and overestimated at a relatively high frequency by Gubernatis's equation. By comparing figures 1, 2 and 3, it can be seen that the deviation among these numerical results obtained by the three equations increase gradually with the increase of the volume fraction. It is also noted that the deviations of the phase velocities predicted by the three equations are larger for the shear wave than for the longitudinal wave. With respect to the effective elastic moduli of the composite material, it can be also seen that the shear moduli predicted by the three equations have more evident deviation than the bulk moduli. The effective attenuations predicted by the three equations have less noticeable deviation at a relatively low concentration. The comparison between equations (21) and (22) is performed and is shown in **figure 4**. It can be seen that the effective phase velocities, effective attenuations and the effective elastic moduli are overestimated by the Gubernatis's equation without iterative process when compare with the prediction by ones with iterative process.

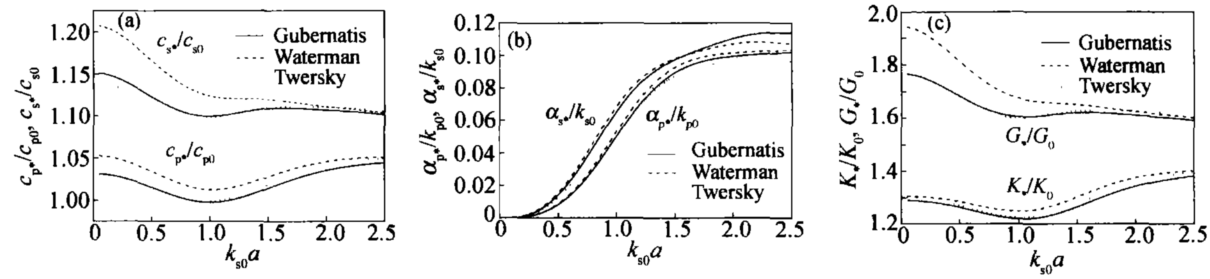

Figure 3 Effective phase velocities, effective attenuations and effective elastic moduli predicted by three coherent plane wave equations at the volume fraction *c*=0.3.

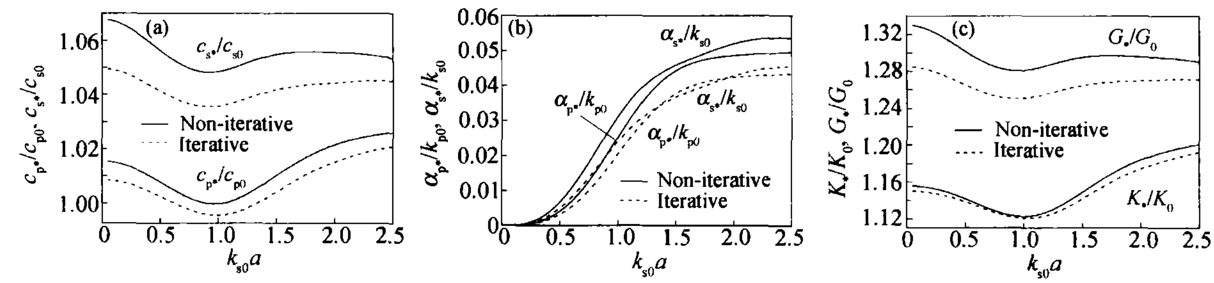

Figure 4 Effective phase velocities, effective attenuations and effective elastic moduli predicted by Gubernatis's equation with and without iteration at the volume fraction c=0.15.

5 Conclusion

Although three coherent plane wave equations, namely, Waterman & Truell's equation, Twersky's equation and Gubernatis's equation, are obtained under the same assumption that the correlation of the positions of scatterers can be neglected, evident deviations arise when they are used to predict the effective properties of a composite material. The deviations among the prediction results are more evident for a shear wave than for a longitudinal wave. Similarly, the deviations among the prediction results are more evident for the effective shear modulus than for the effective bulk modulus. Generally speaking, Twersky's equation and Gubernatis's equation with and without iterative process underestimate the effective phase velocities and the effective elastic moduli when compare with the prediction by Waterman & Truell's equation. However, the deviations decrease gradually with the increase of the frequency and increase gradually with the increase of the volume fraction.

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