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Enhanced group velocity in composite media of particles with non-spherical shape or shape distribution

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Abstract

Effective medium approximation is derived to estimate the effective refractive index n_e and the group velocity v_g in two-phase composites in which one of the components is non-spherical, and even distributed in shape. Enhanced group velocity may be achieved through the suitable adjustment of the particles' shape and shape distribution. The range of the volume fractions, in which the group velocity is enhanced, will expand, once we take into account the non-spherical shape or the shape distribution. Therefore, the non-spherical shape and shape distribution play crucial roles in determining the group velocity in two-phase composites.

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1. Introduction

The physics of inhomogeneous composite materials has been the subject of growing interest over the years because of its potential applications in laser physics and optical technology [1, 2]. Many interesting properties in composite materials have been predicted such as large optical nonlinearity enhancement through the local field effect [3] and the tunability of the group velocity through the adjustment of the dielectric properties of the components [4]. For the latter, Sølna and Milton [5, 6] showed that the planar composite materials, such as superlattices of thin films, can exhibit a larger group velocity of electromagnetic signals than the one in its components, if we combine one component with high refractive index and low dispersion with the other component with low refractive index and high dispersion. More recently, Mackay and Lakhtakia adopted effective medium approximation to deal with enhancement group velocity in granular composite materials, in which both components are spherical in shape and are randomly distributed [7].

It is known that, for real composite materials, the granular inclusions are usually non-spherical and even shape-distributed. In this paper, we aim at studying the effect of both the shape and shape distribution of granular inclusions on the group velocity of electromagnetic signals in two-phase composite materials. According to the suggestion by Bohren and Huffman that spectra of particles of any complicated form may be approximated by the average spectra of ellipsoidal particles [8], we assume that one component is ellipsoidal in shape with the volume fraction p, while the other component is spherical with the volume fraction $q = (1 - p)$. Based on the self-consistent condition of zero net polarizability, we derive effective medium approximation (EMA) to estimate the effective refractive index by taking into account the shape or shape distribution [9–11]. Then, we can take one step forward to investigate the group velocity in such composites. We shall see that the group velocity in the composites can exceed the group velocities in their components by our suitable choice of the particles' shape or shape distribution.

Our paper is organized as follows. In section 2, on the basis of EMA, we establish the formulae for the group velocity in the composite system with shape or shape distribution. In section 3, we present our numerical results. Finally, a summary of our results will be given in section 4.

2. Theoretical development

We consider a two-phase, three-dimensional granular composite, in which the ellipsoidal component 1 with the volume fraction p and the permittivity $\epsilon_1 = n_1^2$, and the spherical component 2 with volume fraction q ($\equiv 1 - p$) and permittivity $\epsilon_2 = n_2^2$, are randomly distributed and randomly oriented (n_i are the refractive indices of the component i; we have assumed that both phases have magnetic permeability $\mu = 1$). According to the definition of the group velocity of a wave packet propagating through each component, one yields [12]

$$v_i = \left. \frac{c}{n_i + \omega \frac{\mathrm{d}n_i}{\mathrm{d}\omega}} \right|_{\omega=\omega_0}, \tag{1}$$

where ω_0 is the centre frequency of the initial wave packet and c is the light speed in the free space. Then, the group velocity in the homogenized composite media can be written as

$$v_{\mathrm{g}} = \left. \frac{c}{n_{\mathrm{e}} + \omega \frac{\mathrm{d}n_{\mathrm{e}}}{\mathrm{d}\omega}} \right|_{\omega=\omega_0}, \tag{2}$$

where n_{e} is the effective refractive index and v_{g} is evaluated at the angular frequency $\omega = \omega_0$. It is evident that the group velocity in composites depends not only on the effective refractive index, but also on its variation with frequency.

We are now in a position to determine n_{e} as a function of the physical parameters of the components such as n_1 and n_2, and the volume fraction p. For this purpose, we consider the embeddings of both components 1 and 2 in a uniform medium, which has an effective refractive index n_{e}. Since the particles are equally oriented, the average over all orientations of the polarizability density produced in the granular inclusions made of component i is of the form [9]

$$\langle P \rangle_i = \frac{n_i^2 - n_{\mathrm{e}}^2}{3} \left[\frac{1}{L_x n_i^2 + (1 - L_x) n_{\mathrm{e}}^2} + \frac{1}{L_y n_i^2 + (1 - L_y) n_{\mathrm{e}}^2} + \frac{1}{L_z n_i^2 + (1 - L_z) n_{\mathrm{e}}^2} \right], \tag{3}$$

where L_j is the ellipsoid depolarization factor along three-symmetric axes and will be used to characterize the shape of the ellipsoids. Note that $L_x + L_y + L_z = 1$ must be satisfied.

Incidentally, for different geometrical configurations of an identical roughing sphere, L can be interpreted as equivalent depolarization factors. For example, one has $L_x = L_y = 0.435$ for the single-strand chain and $L_x = 0.0865$, $L_y = 0.827$ for the fcc lattice [13]. The effective refractive index n_e can then be established by imposing the consistency requirement that the arithmetic average of the polarizability density over different types of granular inclusions vanishes

$$p\langle P\rangle_1 + q\langle P\rangle_2 = 0. \tag{4}$$

As granular inclusions made of component 2 are spherical, equation (4) can be expressed as [11, 13]

$$p\frac{1}{3}\sum_{j=1}^{3}\frac{n_1^2 - n_e^2}{n_e^2 + L_j\left(n_1^2 - n_e^2\right)} + 3(1-p)\frac{n_2^2 - n_e^2}{n_2^2 + 2n_e^2} = 0. \tag{5}$$

Here we would like to mention that in writing the above equations, we have assumed the linear dimension of these particles to be small enough (compared to wavelength λ), so that the quasi-static approximation is applicable. At the same time, the grains should be large enough to exhibit the bulk property. Note that equation (5) can be valid for all volume fractions p from 0 to 1 [9, 11].

First, we investigate the shape effect on the group velocity in the composites v_g. For simplicity, we assume that the ellipsoidal particles are spheroidal in shape and each spheroidal particle possesses the same shape, described by the depolarization factor $L_z \equiv L$ $[L_x = L_y = (1-L)/2]$. As a result, equation (5) reduces to

$$p\left(n_1^2 - n_e^2\right)\left[\frac{1}{n_e^2 + L\left(n_1^2 - n_e^2\right)} + \frac{4}{(1-L)n_1^2 + (1+L)n_e^2}\right] + 9(1-p)\frac{n_2^2 - n_e^2}{n_2^2 + 2n_e^2} = 0. \tag{6}$$

Differentiation of equation (6) with respect to ω yields

$$\frac{\mathrm{d}n_e}{\mathrm{d}\omega} = \rho_1\frac{n_1}{n_e}\frac{\mathrm{d}n_1}{\mathrm{d}\omega} + \rho_2\frac{n_2}{n_e}\frac{\mathrm{d}n_2}{\mathrm{d}\omega}, \tag{7}$$

with

$$\rho_1 = \frac{p\left[8n_e^2/\left[2n_e^2 + (1-L)\left(n_1^2 - n_e^2\right)\right]^2 + n_e^2/\left[n_e^2 + L\left(n_1^2 - n_e^2\right)\right]^2\right]}{p\left[8n_1^2/\left[2n_e^2 + (1-L)\left(n_1^2 - n_e^2\right)\right]^2 + n_1^2/\left[n_e^2 + L\left(n_1^2 - n_e^2\right)\right]^2\right] + 27(1-p)n_2^2/\left(n_2^2 + 2n_e^2\right)^2},$$

$$\rho_2 = \frac{27(1-p)n_e^2/\left(n_2^2 + 2n_e^2\right)^2}{p\left[8n_1^2/\left[2n_e^2 + (1-L)\left(n_1^2 - n_e^2\right)\right]^2 + n_1^2/\left[n_e^2 + L\left(n_1^2 - n_e^2\right)\right]^2\right] + 27(1-p)n_2^2/\left(n_2^2 + 2n_e^2\right)^2}.$$

Equations (6), (7) and (2) allow us to control the group velocity by changing the particles' shape.

Next, we take one step forward to investigate the effect of shape distribution on the group velocity in the composites. For an assembly of component 1 having different ellipsoidal shapes, $\langle P\rangle_1$ in equation (3) is generalized to be [14, 15]

$$\langle P\rangle_1 = \frac{n_1^2 - n_e^2}{3}\iint\left[\frac{1}{L_x n_1^2 + (1-L_x)n_e^2} + \frac{1}{L_y n_1^2 + (1-L_y)n_e^2} + \frac{1}{(1-L_x-L_y)n_1^2 + (L_x+L_y)n_e^2}\right] f(L_x, L_y)\,\mathrm{d}L_x\,\mathrm{d}L_y, \tag{8}$$

where $f(L_x, L_y)$ is the distribution function of the depolarization factor, which can in principle, be used to describe the shape distribution. Here we assume the shape distribution function to be [16]

$$f(L_x, L_y) = C\Theta\left(L_x - \frac{1}{3} + \frac{\Delta}{3}\right)\Theta\left(L_y - \frac{1}{3} + \frac{\Delta}{3}\right)\Theta\left(\frac{2}{3} + \frac{\Delta}{3} - L_x - L_y\right), \qquad (9)$$

where $C = 2/\Delta^2$ is the normalized constant and $\Theta(\cdot)$ is the Heaviside function. Moreover, Δ is the shape variance parameter of the granular inclusions made of component 1, which defines both the domain of nonzero values and the half-width of the $f(L_x, L_y)$ function. Equation (9) indicates that deviations of particle shape from spherical to ellipsoidal are considered to be equiprobable. As a matter of fact, Δ can change from zero to unity. Physically, for $\Delta = 0$, all granular inclusions are spherical in shape ($L_j = 1/3$ for $j = 1, 2, 3$), and for $\Delta = 1$, all possible ellipsoidal shapes are equiprobable [16]. Substituting equation (9) in (8), one has

$$\langle P\rangle_1 = \frac{2}{\Delta^2}\left[\left(\frac{n_e^2}{n_1^2 - n_e^2} + \frac{1+2\Delta}{3}\right)\ln\left(\frac{n_e^2/\left(n_1^2 - n_e^2\right) + (1+2\Delta)/3}{n_e^2/\left(n_1^2 - n_e^2\right) + (1-\Delta)/3}\right) - \Delta\right]. \qquad (10)$$

The self-consistency equation (4) can then be written as

$$\frac{2p}{\Delta^2}\left[\left(\frac{n_e^2}{n_1^2 - n_e^2} + \frac{1+2\Delta}{3}\right)\ln\left(\frac{n_e^2/\left(n_1^2 - n_e^2\right) + (1+2\Delta)/3}{n_e^2/\left(n_1^2 - n_e^2\right) + (1-\Delta)/3}\right) - \Delta\right] + 3(1-p)\frac{n_2^2 - n_e^2}{n_2^2 + 2n_e^2} = 0. \qquad (11)$$

Equation (11) is effective medium approximation with shape distribution, which will be used to estimate the effective refractive index of the random mixture in which the first component possesses the shape distribution form, described by equation (9). Similar to the above process, one obtains

$$\frac{dn_e}{d\omega} = \kappa_1\frac{n_1}{n_e}\frac{dn_1}{d\omega} + \kappa_2\frac{n_2}{n_e}\frac{dn_2}{d\omega}, \qquad (12)$$

with

$$\kappa_1 = \frac{2p[\ln(A/B) - \Delta/B]n_e^2/\left(n_1^2 - n_e^2\right)^2}{2p[\ln(A/B) - \Delta/B]n_1^2/\left(n_1^2 - n_e^2\right)^2 - 9(1-p)\Delta^2 n_2^2/\left(n_2^2 + 2n_e^2\right)^2},$$

$$\kappa_2 = \frac{-9(1-p)\Delta^2 n_e^2/\left(n_2^2 + 2n_e^2\right)^2}{2p[\ln(A/B) - \Delta/B]n_1^2/\left(n_1^2 - n_e^2\right)^2 - 9(1-p)\Delta^2 n_2^2/\left(n_2^2 + 2n_e^2\right)^2},$$

where $A = n_e^2/\left(n_1^2 - n_e^2\right) + (1+2\Delta)/3$ and $B = n_e^2/\left(n_1^2 - n_e^2\right) + (1-\Delta)/3$.

3. Numerical results

For numerical calculations, we choose $n_1 = 20$ and $n_2 = 1.2$. Moreover, to observe the enhanced group velocity easily, we set $\frac{dn_1}{d\omega}\big|_{\omega=\omega_0} = \frac{1}{\omega_0}$ and $\frac{dn_2}{d\omega}\big|_{\omega=\omega_0} = \frac{20}{\omega_0}$.

In figure 1, we plot the group velocity v_g against the volume fraction p in composite materials consisting of spheroidal particles with various L. It is evident that the group velocity v_g in the composite can exceed group velocities in both components in certain volume fraction regions, dependent on the shape of the spheroidal particles. For instance, when both components are spherical in shape, i.e. $L = 1/3$, one has $v_g > v_i$ ($i = 1, 2$) for $0.41 < p < 1$. To one's interest, when the granular shape deviates from the spherical one, the volume fraction range corresponding to the enhanced group velocity will be enlarged regardless of the prolate ($L < 1/3$) or oblate ($L > 1/3$) one. Actually, for both needle-shape ($L = 0$) and disc-shape

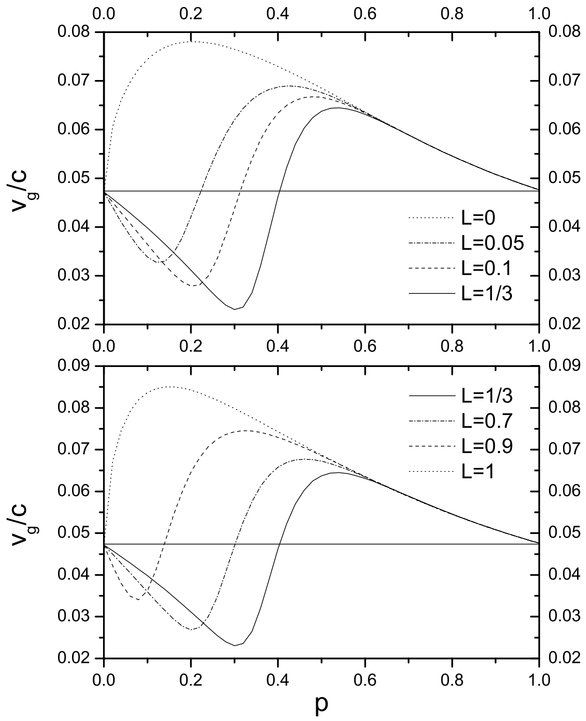

Figure 1. The group velocity v_g in composite materials plotted against the volume fraction p for various depolarization factors L with equations (6), (7) and (2). Note that the group velocities in components are almost equal to each other.

($L = 1$), the fraction region in which $v_g > v_1$ (and v_2) lies in the whole range from 0 to 1. For large volume fractions, the spheroidal particles made of component 1 always form an infinite cluster through the whole system and the percolation effect arises. As a result, the group velocity in the composites exhibits no dependence on the depolarization factors for large p. In addition, in the composite media consisting of spherical inclusions ($L = 1/3$), one has the maximal group velocity $v_{g,max}$ at $p_{max} \approx 0.54$ and the minimal one $v_{g,min}$ at $p_{min} \approx 0.31$. With the variation of the depolarization factor from 1/3 to 0 (or 1), we predict that p_{max} shifts to low volume fraction, accompanied with the increase of the maximal group velocity. This is clearly shown in figure 2. Therefore, we conclude that the adjustment of the particle's shape from the spherical one is indeed helpful to realize the enhanced group velocity in composites. To achieve the maximal group velocity, the use of the oblate spheroidal particles is more prominent than the use of prolate inclusions.

Finally, we study the effect of shape distribution on the group velocity in the composites. Numerical results are shown in figure 3. The shape distribution is also found to play an important role in determining the group velocity in the composites. With increasing Δ from $\Delta = 0$ (all particles are spherical in shape) to $\Delta = 1$ (all possible ellipsoids exist), the fraction region corresponding to enhanced velocity expands as expected. For instance, we have enhanced v_g in the region $p = 0.41$–1.0 for $\Delta = 0$ and in the region $p = 0.23$–1.0 for $\Delta = 1$. Furthermore, from figure 4, we observe that the maximal group velocity $v_{g,max}$ exhibits monotonic increase and its position exhibits the shifts to small volume fractions with increasing Δ.

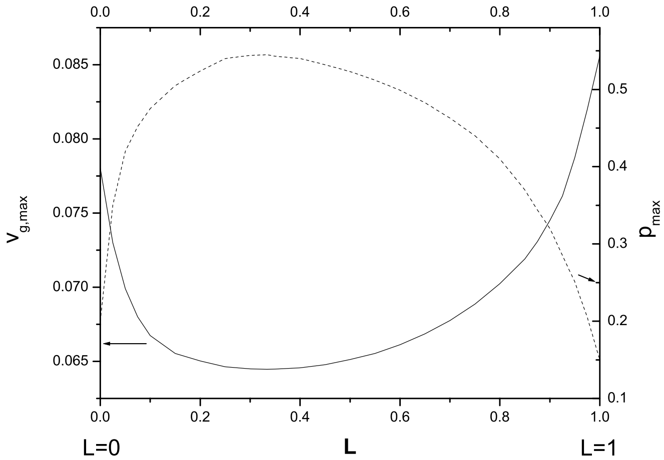

Figure 2. The peak value of group velocity and the corresponding volume fraction against the depolarization factor *L*.

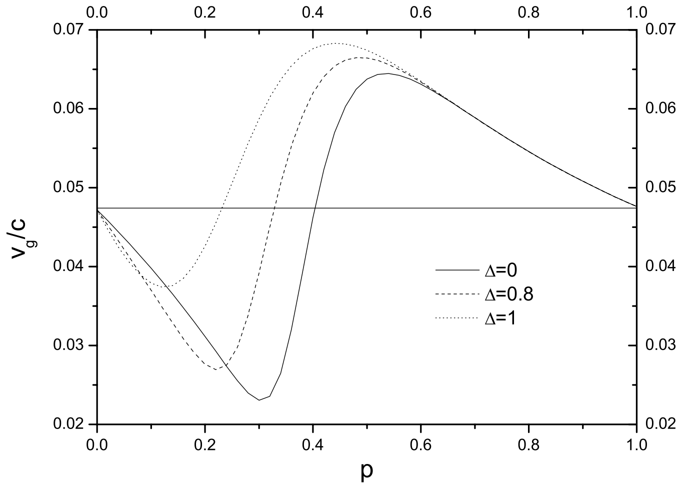

Figure 3. The plot of v_g against p for various shape distribution parameters Δ with equations (11), (12) and (2).

4. Summary

In this paper, with the aid of effective medium approximation, we have found that the introduction of the non-spherical shape and shape distribution is helpful to obtain enhanced group velocity and to expand the range of volume fraction corresponding to the enhanced group velocity. The maximal group velocity in the composite system can be achieved at a certain volume fraction p_c, which is strongly dependent on the particles' shape and shape distribution. As a result, we may get a maximal value of group velocity by taking into account the shape and shape distribution.

Here, some comments are in order. Due to simplistic treatments of the distributional statistics of the components, our formalisms do not include the effect of the scattering losses.

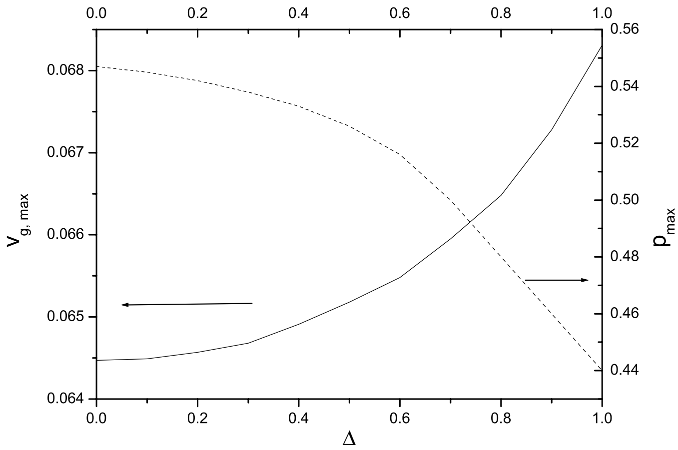

Figure 4. The peak value of group velocity and the corresponding volume fraction of the shaped component against shape variance parameter Δ.

To take into account the scattering losses on the group velocity, some sophisticated approaches, such as those provided by the strong-property-fluctuation theory [17], can be applied.

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