

EFFECTS OF MICROSTRUCTURE ON THE SPEED AND ATTENUATION OF ELASTIC WAVES: FORMAL THEORY AND SIMPLE APPROXIMATIONS

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INTRODUCTION

The sensitivity of the propagation of an elastic wave to changes in the microstructural details of a material is well known.¹ In particular, numerous experiments have shown that the attenuation of the wave is sensitive to the inclusions, voids, cracks, grain boundaries, twin boundaries, interphase boundaries, magnetic domain walls, dislocations, substitutional impurities of a material. For attenuation studies in metals, ceramics and polycrystals, three formulas, each for different wavelength regimes, are generally used in the quantitative interpretation of experimental results.¹⁻³ If λ is the wavelength of the elastic wave and $\langle D \rangle$ is the average grain diameter, then in the Rayleigh regime ($\lambda \gg D$), $\alpha = A_1 \langle D \rangle^3 \lambda^4$, in the stochastic regime ($\lambda \simeq D$), $\alpha = A_2 \langle D \rangle \lambda^2$, and in the diffusive regime ($\lambda \ll D$), $\alpha = A_3 / \langle D \rangle^{-1}$. By fitting the data to these formulas, one tries to infer $\langle D \rangle$.

In practice, however, these formulas prove to be only semi-quantitative since the measurements seldom exhibit the indicated power law behaviors for λ .³ Additionally, they are not the only formulas used. For example, in the Rayleigh regime, relations such as $\alpha = A_1 \langle D^3 \rangle \lambda^4$ and $\alpha = A_1 \langle D^6 \rangle \lambda^4 / \langle D^3 \rangle$ are also used. Since $\langle D^n \rangle \neq \langle D \rangle^n$ and since usually $\langle D^{2n} \rangle / \langle D^n \rangle \gg \langle D^n \rangle$, a variety of quantitative predictions on the same data are possible.

Recently, there have been several attempts at a more unified theory of the attenuation and its relation to microstructure statistics.^{4,5} The work with a clear applicability to elastic wave

propagation is that by Evans et al.⁴ who assume the attenuation equals $n\bar{\sigma}$ where n is the density of scatterers and $\bar{\sigma}$ is the total cross section of a scatterer averaged over the distribution of scatterers. Using the experimentally determined grain distribution, they obtained good agreement between theory and experiment.

In this paper, we also discuss a unified theory. But in contrast to nearly all previous treatments we follow a first principles approach, using developments from other multiple scattering problems and adapting them to the elastic wave case. We then present several simple, standard approximations. In the process we will clarify the validity of the commonly made assumption that $\alpha = n\bar{\sigma}$, and will also compute the effective speed, illustrating its complementary character to the attenuation. Our principal objective is to present the formal analysis necessary to treat systematically the dependency of the wave propagation on microstructural statistics.

FORMAL ASPECTS

The displacement field $u_i(\vec{r})$ associated with propagation of an elastic wave through an inhomogeneous material, described by a density $\rho(\vec{r})$ and elastic stiffness $C_{ijkl}(\vec{r})$, obeys the integral equation^{6,7}

$$u_i(\vec{r}) = u_i^o(\vec{r}) + \int d\vec{r}' g_{ij}^o(\vec{r}-\vec{r}') v_{jk}(\vec{r}') u_k(\vec{r}') \quad (1)$$

in which all the details about the inhomogeneity are contained in

$$v_{ij}(\vec{r}) = \delta\rho(\vec{r})\omega^2\delta_{ij} + \frac{\partial}{\partial x_k} \delta C_{ikj\ell}(\vec{r}) \frac{\partial}{\partial x_\ell} \quad (2)$$

The fields $\delta\rho(\vec{r})$ and $\delta C_{ijkl}(\vec{r})$ are defined relative to homogeneous fields ρ^o and C_{ijkl}^o ,

$$\delta\rho(\vec{r}) = \rho(\vec{r}) - \rho^o$$

$$\delta C_{ijkl}(\vec{r}) = C_{ijkl}(\vec{r}) - C_{ijkl}^o$$

These homogeneous fields are arbitrary, but often are chosen to be the average density $\langle\rho(\vec{r})\rangle$ and average elastic stiffness $\langle C_{ijkl}(\vec{r})\rangle$ or the density and elastic stiffness of an embedding medium. The functions $u_i^o(\vec{r})$ and $g_{ij}^o(\vec{r}-\vec{r}')$ are the displacement field and Green's function for the homogeneous material:

$$C_{ijkl}^o u_{k,lj}^o + \rho^o \omega^2 u_i^o = 0 \quad (3)$$

and

$$C_{ijkl}^o g_{mk,lj}^o + \rho^o \omega^2 g_{im}^o + \delta_{im} \delta(\vec{r}-\vec{r}') = 0 \quad (4)$$

We take C_{ijkl}^o to be isotropic and defined by the Lamé parameters λ^o and μ^o . Also

$$u_i^o = \hat{a}_i e^{i\vec{k}^o \cdot \vec{r}} = \hat{a}_i e^{i\vec{k}^o \hat{k} \cdot \vec{n}}$$

where \hat{a}_i is a unit vector and k_i equals α_o (or β_o) for longitudinal (shear) waves. For an unbounded isotropic material,^{6,7}

$$g_{ij}^o = \frac{1}{4\pi\rho^o\omega^2} \left[\delta_{ij}\beta_o^2 \frac{e^{i\beta_o R}}{R} + \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} \left(\frac{e^{i\alpha_o R}}{R} - \frac{e^{i\beta_o R}}{R} \right) \right] \quad (5)$$

where

$$\alpha_o^2 = (\lambda^o + 2\mu)/\rho^o \quad , \quad (6a)$$

$$\beta_o^2 = \mu^o/\rho^o \quad . \quad (6b)$$

It is convenient to rewrite (3) as

$$L_{ij}^o(\vec{k}^o) u_j^o = 0 \quad (7)$$

with

$$L_{ij}^o(\vec{k}) \equiv (\lambda^o + \mu^o) k_i k_j + (\mu^o k^2 - \rho^o \omega^2) \delta_{ij} \quad . \quad (8)$$

The basic problem is to find $\langle u_i(\vec{r}) \rangle$ from (1). More specifically, since $\langle u_i \rangle = \hat{a}_i e^{i\vec{k} \cdot \vec{r}} = \hat{a}_i e^{i\vec{k} \hat{k} \cdot \vec{r}}$, the problem is to find \vec{k} . To do so requires finding a new operator $K_{ij}(\vec{k})$, the effective wave number operator,⁸ such that $\langle u_i \rangle$ satisfies

$$\left[L_{ij}^0(\vec{k}) + K_{ij}(k) \right] \langle u_j \rangle = 0 \quad . \quad (9)$$

In general $K_{ij}(k)$ will be a complex number whose real part is related to the shift in phase velocity of the incident wave and whose imaginary part is related to the attenuation.

For compactness in the development of our formal analysis, we rewrite (1), (4) and (7) in an operator notation

$$L^0 u^0 = 0 \quad ,$$

$$L^0 g^0 + I = 0 \quad ,$$

$$u = u^0 - g^0 v u \quad .$$

Then, by use of the scattering operator T defined by

$$T u^0 = v u \quad (10)$$

we rewrite (1) as

$$u = u^0 + g^0 T u^0 \quad (11)$$

so the average field is simply given by

$$\langle u \rangle = u^0 + g^0 \langle T \rangle u^0 \quad .$$

But from this equation it follows that

$$u^0 = (I - g^0 \langle T \rangle)^{-1} \langle u \rangle \quad . \quad (12)$$

Therefore, we can write an integral equation for $\langle u \rangle$

$$\langle u \rangle = u^0 + g^0 K \langle u \rangle \quad , \quad (13a)$$

where

$$K = \langle T \rangle (I + g^0 \langle T \rangle)^{-1} \quad . \quad (13b)$$

Operating with L^0 on both sides of (13a) reduces it to the desired form; namely,

$$(L^0 + K)\langle u \rangle = 0 \quad . \quad (13c)$$

Since (3b) can be rewritten as

$$\langle T \rangle = K(I - g^0 K)^{-1} \quad ,$$

we note that for a k satisfying $I - g^0 K(k) = 0$ the $\langle T \rangle$ matrix has a pole, and, at the same time, (13c) is satisfied. Thus finding a (complex) k value for which (13c) has a plane wave solution is equivalent to locating a pole of $\langle T \rangle$.

With the re-introduction of subscripts and arguments, (7) is

$$\left[L_{ij}^0(\vec{k}) + K_{ij}(k) \right] \hat{a}_j e^{i\vec{k} \cdot \vec{r}} = 0 \quad .$$

If $\langle u_i \rangle$ is longitudinal ($\hat{a}_i = \hat{k}_i$), this equation is equivalent to

$$k^2 = \alpha_0^2 + (\lambda^0 + 2\mu^0)^{-1} K_{ij}(k) \hat{k}_i \hat{k}_j \quad (14a)$$

If $\langle u_i \rangle$ is transverse ($\hat{a}_i = \hat{k}_i$ and $\hat{k}_i \hat{k}_i = 0$), then the equation is equivalent to

$$k^2 = \beta_0^2 + (\mu^0)^{-1} K_{ij}(k) \hat{k}_i \hat{k}_j \quad (14b)$$

Hence, the basic problem can now be stated as evaluating the function $K_{ij}(k)$ and solving (14) for k .

Evaluating $K_{ij}(k)$ is easier said than done. Finding suitable approximations to K_{ij} is a more proper statement of the task at hand. A convenient, systematic way to approximate K_{ij} is to expand the power series in (13). Before doing so, we first rewrite T in the standard multiple scattering form⁹

$$T = \sum_a t^\alpha + \sum_\alpha \sum_{\beta \neq \alpha} t^\alpha g^0 t^\beta + \sum_\alpha \sum_{\beta \neq \alpha} \sum_{\gamma \neq \beta} t^\alpha g^0 t^\beta g^0 t^\gamma + \dots$$

where t^α is the scattering operator for an individual scatterer (a grain, void, etc.). Then by inserting T into (13) and expanding the power series, we find that

$$K = K^{(1)} + K^{(2)} + K^{(3)} + \dots \quad (15)$$

where

$$K^{(1)} = \langle \sum_{\alpha} t^{\alpha} \rangle \quad (16a)$$

$$K^{(2)} = \langle \sum_{\alpha} \sum_{\beta \neq \alpha} t^{\alpha} g^{\circ} t^{\beta} \rangle - \langle \sum_{\alpha} t^{\alpha} \rangle g^{\circ} \langle \sum_{\alpha} t^{\alpha} \rangle \quad (16b)$$

$$K^{(3)} = \langle \sum_{\alpha} \sum_{\beta \neq \alpha} \sum_{\gamma \neq \beta} t^{\alpha} g^{\circ} t^{\beta} g^{\circ} t^{\gamma} \rangle - \langle \sum_{\alpha} \sum_{\beta \neq \alpha} t^{\alpha} g^{\circ} t^{\beta} \rangle g^{\circ} \langle \sum_{\alpha} t^{\alpha} \rangle \quad (16c)$$

$$- \langle \sum_{\alpha} t^{\alpha} \rangle g^{\circ} \langle \sum_{\alpha} \sum_{\beta \neq \alpha} t^{\alpha} g^{\circ} t^{\beta} \rangle + \langle \sum_{\alpha} t^{\alpha} \rangle g^{\circ} \langle \sum_{\alpha} t^{\alpha} \rangle g^{\circ} \langle \sum_{\alpha} t^{\alpha} \rangle$$

etc.

These expressions have the feature of establishing a hierarchy for the statistical information required to evaluate the series. For example, the evaluation of the third term requires the first three statistical correlation functions, but not the fourth.

SIMPLE APPROXIMATIONS

The simplest approximation is

$$K \simeq K^{(1)} = \langle \sum_{\alpha} t^{\alpha} \rangle \quad (17)$$

Regarding α as statistical variable, we write

$$K = \int d\alpha P(\alpha) t(\alpha) \equiv n \bar{t}$$

where $P(\alpha)$ is the probability of finding a scatterer with the properties denoted by α (grain size, shape, orientation, etc.). The basic equation to be solved becomes

$$k^2 = \alpha_o^2 + (\lambda^{\circ} + 2\mu^{\circ})^{-1} n \bar{t}_{ij}(k) \hat{k}_i \hat{k}_j \quad (18a)$$

or

$$k^2 = \beta_0^2 + (\mu^0)^{-1} n \bar{t}_{ij}(k) \hat{k}_i \hat{k}_j \quad . \quad (18b)$$

The single-site scattering operator bears a simple relation to the scattered amplitude. To establish it, one starts with (10)

$$t_{ij}(\vec{r}) \hat{a}_j e^{i\vec{k}_0 \cdot \vec{r}} = v_{ij}(\vec{r}) u_j(\vec{r}) \quad ,$$

multiplies both sides by $\hat{a}_i e^{-i\vec{k} \cdot \vec{r}}$ and then integrates both sides over all space to find

$$\begin{aligned} \hat{a}_i \hat{a}_j \int d\vec{r} e^{-i\vec{k} \cdot \vec{r}} t_{ij}(\vec{r}) e^{+i\vec{k}_0 \cdot \vec{r}} \\ = \hat{a}_i \int d\vec{r} e^{-i\vec{k} \cdot \vec{r}} v_{ij}(\vec{r}) u_j(\vec{r}) \quad . \end{aligned}$$

If $\hat{a}_i = \hat{k}_i$, then^{6,7}

$$\hat{k}_i \hat{k}_j t_{ij}(k) = \frac{4\pi\rho\omega^2}{\alpha_0^2} A(k)$$

where $A(k)$ is the longitudinal, forward scattered amplitude. If $\hat{a}_i = \hat{k}_i$ and $\hat{k}_i \hat{k}_i = 0$, then

$$\hat{k}_i \hat{k}_j t_{ij}(k) = \frac{4\pi\rho\omega^2}{\beta_0^2} B(k)$$

where $B(k)$ is transverse, forward scattered amplitude. Hence, (16) reduces to

$$k^2 = \alpha_0^2 + 4\pi n \bar{A}(k) \quad , \quad (19a)$$

and

$$k^2 = \beta_0^2 + 4\pi n \bar{B}(k) \quad . \quad (19b)$$

For compactness we will replace these two equations by

$$k^2 = k_0^2 + 4\pi n \bar{f}(k) \quad . \quad (20)$$

In the context of multiple scattering of scalar waves, the approximation embodied in (20) was first proposed by Foldy¹⁰; later, Lax¹¹ named it the quasi-crystalline approximation. From (16) and (17) one sees that the approximation clearly neglects correlations among the individual scatterers. This approximation has been used by various investigators in elastodynamic effective medium problems.¹² Recently, attempts to go beyond this approximation have been made, but have been restricted to the Rayleigh regime.¹³⁻¹⁵

Often the solution to this equation is approximated by

$$k^2 = k_0^2 + 4\pi n \bar{f}(k_0) \quad (21)$$

and even further approximated by

$$k = k_0 + \frac{2n \operatorname{Re}\{\bar{f}\}}{k_0} + \frac{i2n \operatorname{Im}\{\bar{f}\}}{k_0} \quad . \quad (22)$$

By use of the optical theorem

$$\sigma = \frac{4\pi \operatorname{Im}\{f\}}{k_0} \quad .$$

From the imaginary part of k , the attenuation of power becomes

$$\alpha = 2 \operatorname{Im}\{k\} = n \bar{\sigma} \quad . \quad (23)$$

Thus, we see that the validity of (23) requires small correlations among the scatterers (to justify (17)) and

$$\frac{4\pi n |\bar{f}|}{k_0} \ll k_0 \quad (24)$$

(to justify (22)). Since $|f| > \operatorname{Im}\{f\} \geq 0$, we can re-interpret (25) as

$$\alpha \ll k_0 \quad (26)$$

i.e., the attenuation over a wavelength is small.

CALCULATIONS AND CONCLUSIONS

We have solved (20) and (21) for the effective phase velocity and attenuation for an inhomogeneous material modelled by randomly positioned spherical pores in stainless steel as a function of $k a$ and the porosity, c . In Fig. 1 the results are shown for (21) as a function of 5 evenly distributed values of c between .01 and .05. The attenuation, when divided by $k c$, is seen to be a nearly universal function of $k a$: beyond $k a = 1$, the curves coincide, and below $k a = 1$, the curves nearly coincide as they exhibit only slight displacements from one another. The sensitivity of the phase velocity to c and $k a$ is restricted to $k a < 3$ and is very weak. As seen in Fig. 2, solving the more rigorous approximation (20) produces nearly the same results, the principal difference being a small increase in the displacement of the attenuation curves for $k a < 1$. The coincidence of the curves for $k a > 1$ remains, and the curves for practical purposes are identical to those obtained by solving (21). Solutions of (20) and (21) for $k a$ up to 10 and c up to 0.25 exhibit the same features as just described. For high c , the minimum in phase velocity around $k a = .5$ is more pronounced. The existence of a minimum in phase velocity is consistent with the results of Sayers and Smith.¹⁵

Next, we examined the sensitivity of these features by fixing the porosity, $c = 4\pi \langle a^3 \rangle N/3V$, but varying the radii according to a distribution law. For the distribution law we chose the log-normal function,

$$\beta P(a) = \frac{\beta}{a} \frac{e^{-(\ln \beta/a)^2/2\delta^2}}{\delta\sqrt{2\pi}}$$

which has a characteristic length, β , and has its width and skewness controlled by δ . As shown in Fig. 3, for small δ the distribution is sharply peaked and nearly symmetrical about $\beta/a = 1$, but for large δ the peak moves to smaller values of β/a and becomes very unsymmetrical about the peak values. For this distributed radii model we only solved (21), the less rigorous result. The results are shown in Figs. 4 and 5 for $c = 0.01, 0.03$, and 0.05 . In Fig. 4, $\delta = .01$, which is a sharply-peaked distribution about $\beta = a$; hence, as one would expect, the results are identical to Fig. 1. When $\delta = .1$, modest variation about $\beta = a$ occur, but as shown in Fig. 5, the previously discussed general features are unaltered. In fact, the only mentionable difference between Figs. 1, 4, and 5 is a slight displacement downward ($\approx 5\%$) of the large $k a$ tail in the attenuation curve of Fig. 5.

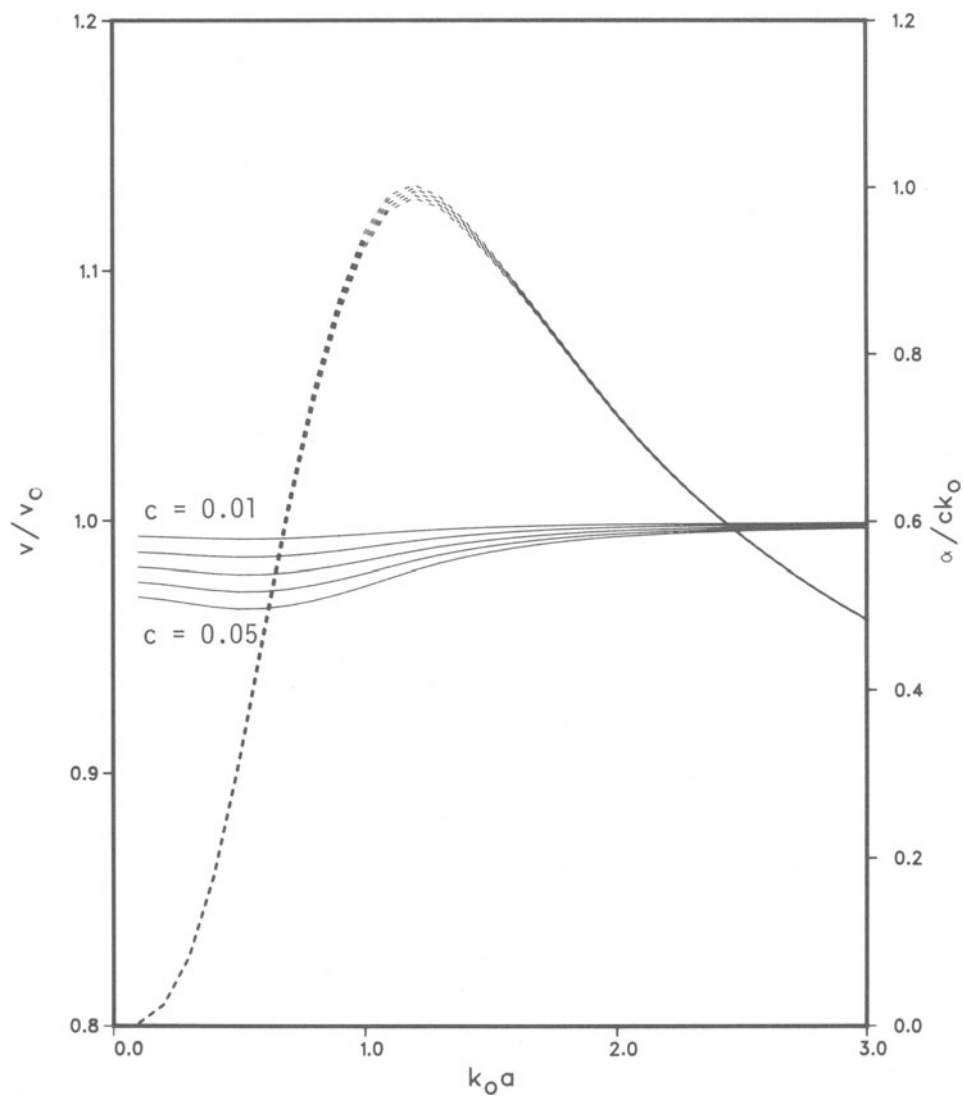


Fig. 1 The prediction of (21) for the relative phase velocity and scaled attenuation (dashed curves) for spherical pores of identical radius as a function of $k_0 a$ and c . The pore radius is a ; the porosity is c ; and the wave-number of the host is k_0 . The porosity varies from 0.01 to 0.05 in steps of 0.01.

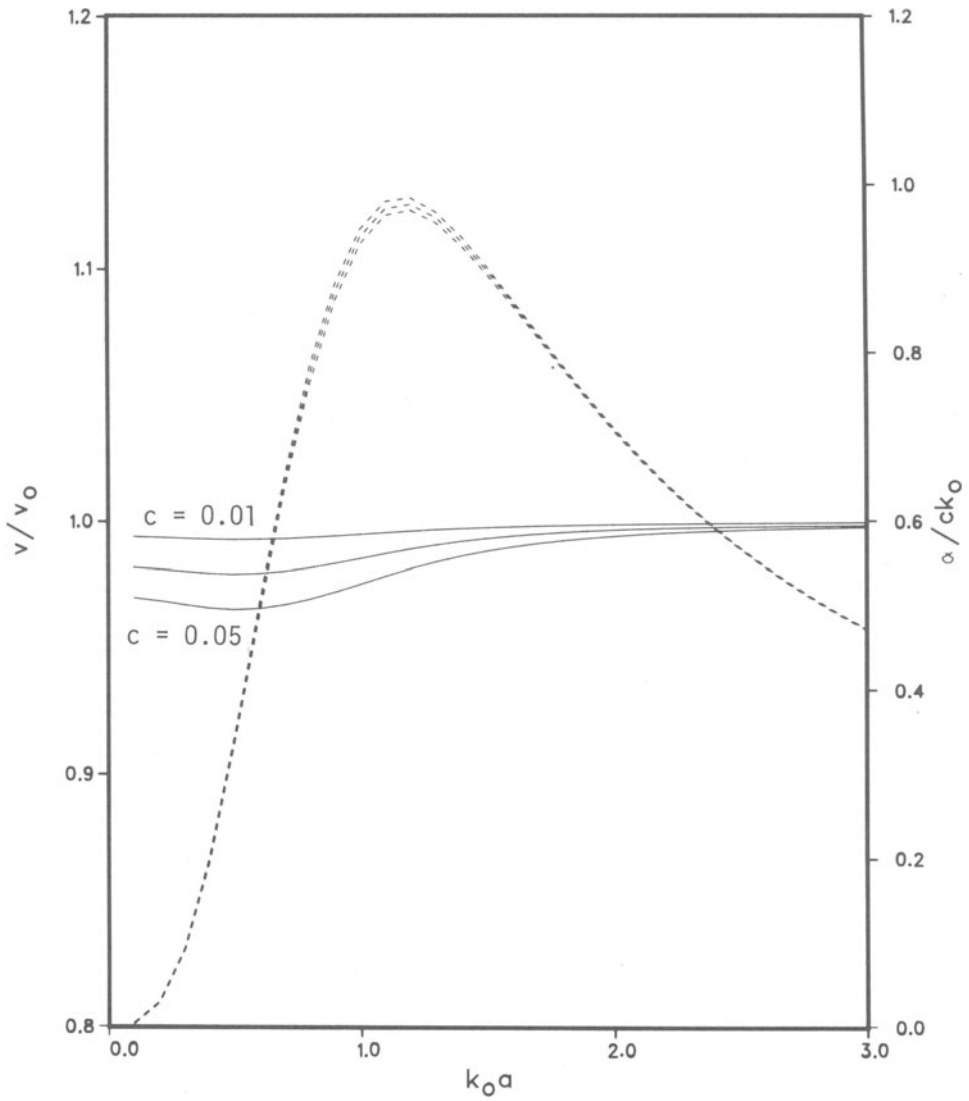


Fig. 2 The predictions of (20) for the relative phase velocity and sealed attenuation (dashed curves) for spherical pores of identical radius as a function of $k_0 a$ and c . The pore radius is a ; the porosity is c ; and the wavenumber of the host is k_0 . The porosity varies from 0.01 to 0.05 in steps of 0.01.

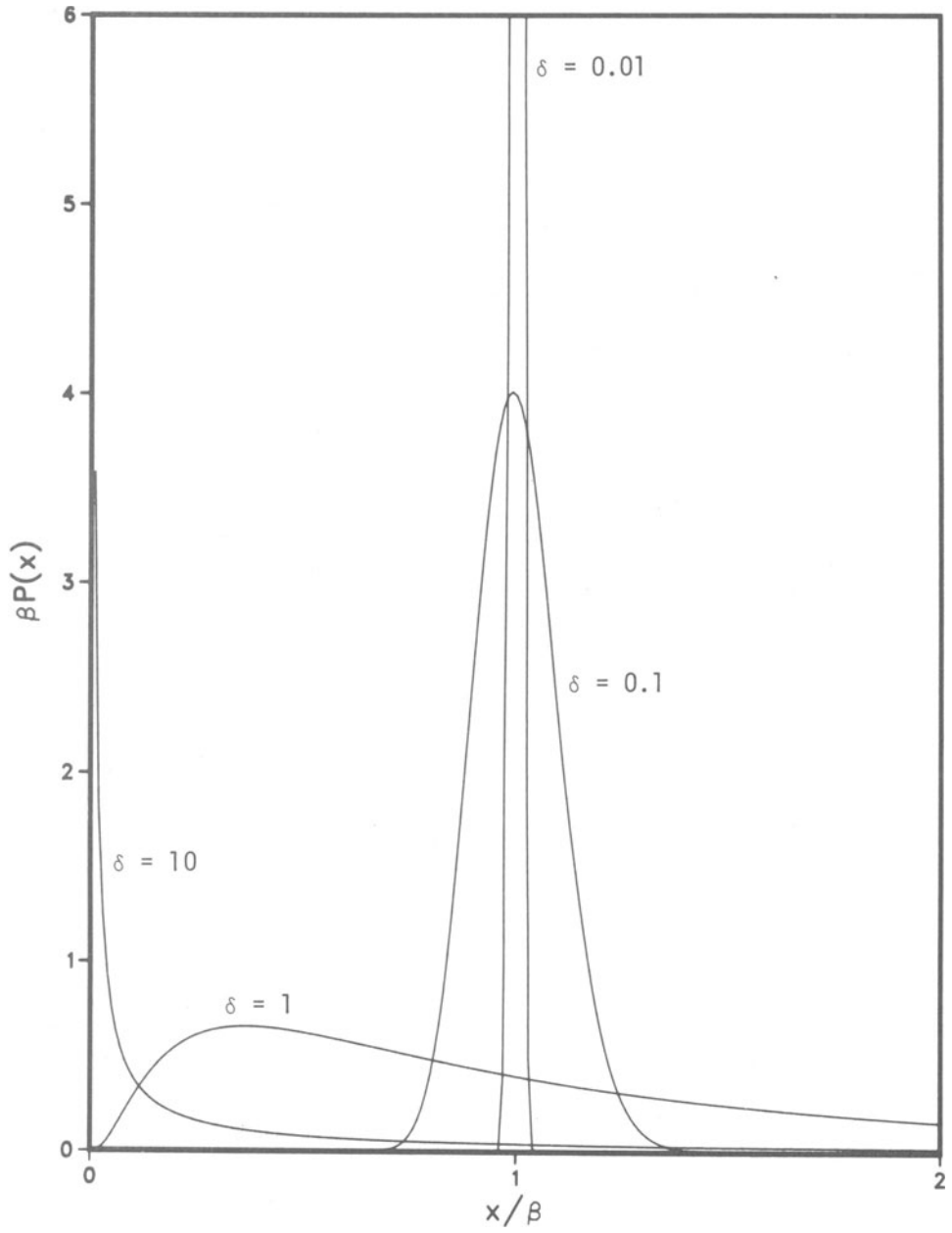


Fig. 3 The log-normal distribution function for various values of δ .

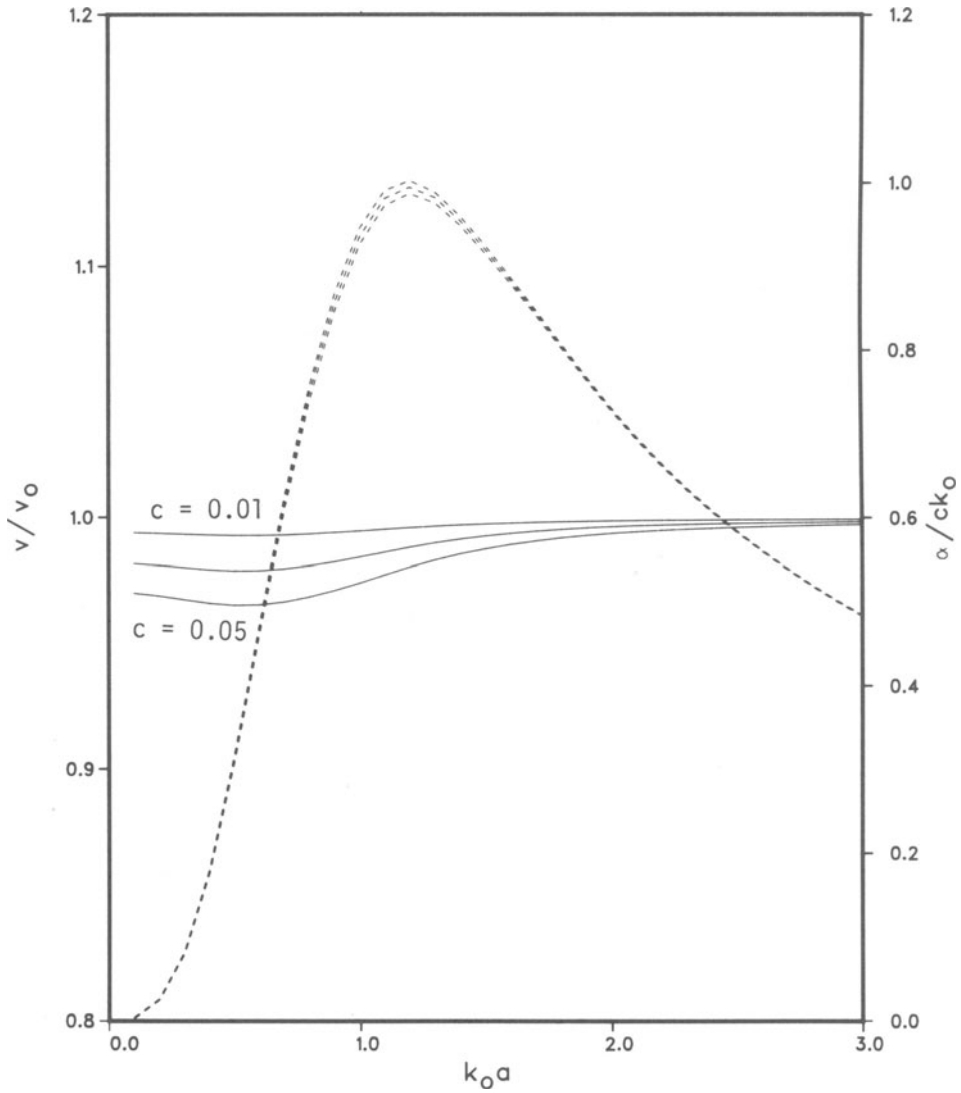


Fig. 4 The predictions of (21) for the relative phase velocity and scaled attenuation (dashed curves) for spherical pores with log-normal distributed radii as a function of $k_0 a$ and c . The porosity $c = 4\pi \langle a^3 \rangle N / 3V$ and equals 0.01, 0.03 and 0.5. $\delta = 0.01$.

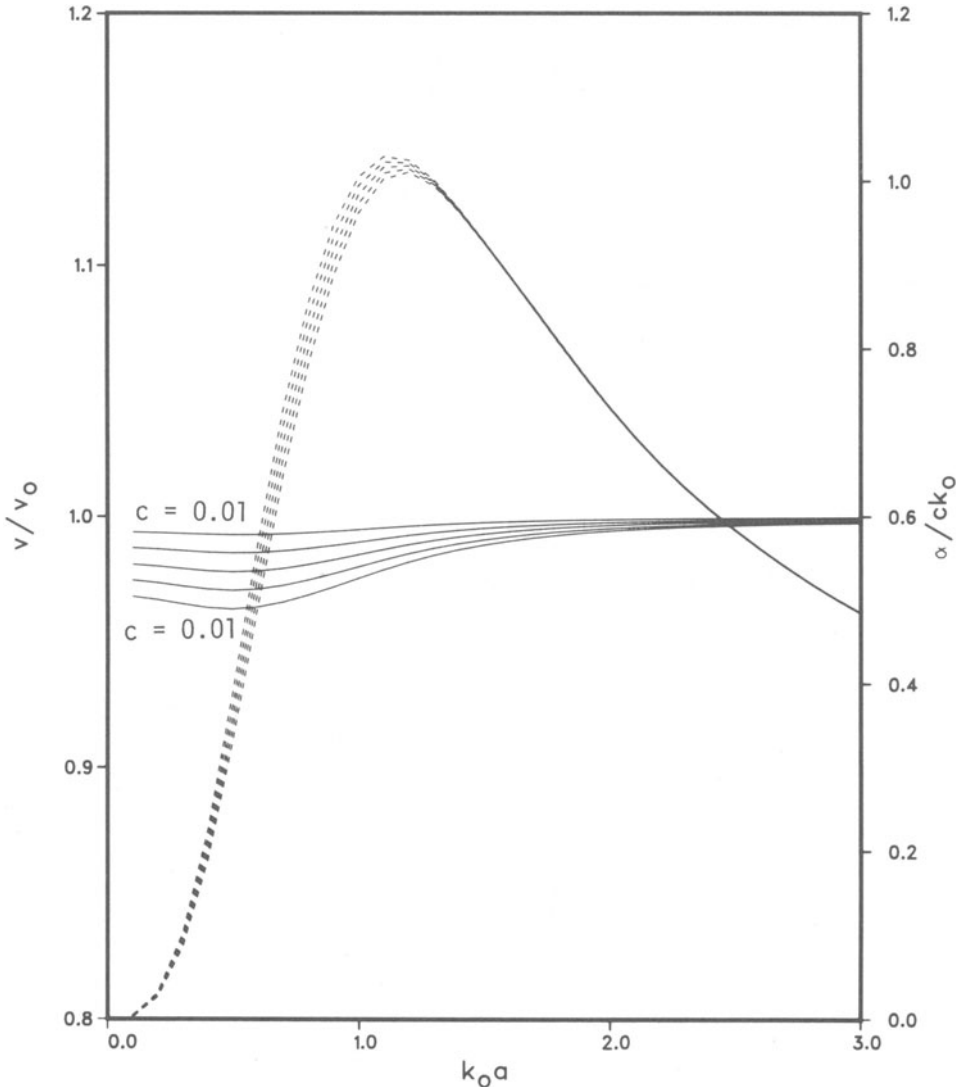


Fig. 5 The predictions of (21) for the relative phase velocity and scaled attenuation (dashed curves) for spherical pores with log-normal distributed radii as a function of $k_0 a$ and c . The porosity $c = 4\pi\langle a^3 \rangle N/3V$ and equals 0.01, 0.03 and 0.5. $\delta = 0.1$.

From the calculations completed to-date, all based on the independent scatterer approximation, there appear to be three basic conclusions: the attenuation, when appropriately scaled, exhibits a nearly universal behavior; the phase velocity is less sensitive than the attenuation to variations of k , a and c ; and both v and α are insensitive to modest variations in pore radius. The nearly universal behavior exhibited by the attenuation suggests a simple procedure for estimating the average pore size and porosity: If α/k is plotted as a function of k_0^{-1} , the value of k_0^{-1} at which the curve peaks is the average size and the inverse of proportionality constant between the experimental curve and the universal curve is the porosity. Of course, this procedure is valid only when the independent scatterer approximation is valid. In addition, the sensitivity of the "universal" features to larger variation in pore radius needs investigation.

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DISCUSSION

- A. Nayfeh (University of Cincinnati): There is a tremendous amount of work which has been done on periodic media in, for example, wave propagation in fibrous composites and layered media. Since you have this model, did you try to see what you would predict for attenuation in periodic media? My understanding is that attenuation will only occur if you have randomness; if you have periodic structures, you don't have any attenuation at all. At the same time, if you go into the very low frequency regime you get the law of mixtures. If you have very high frequencies, then you will see both components of the mixture.
- J.E. Gubernatis (Los Alamos National Laboratory): No, we have not looked at the periodic case. If it is periodic, it's not going to attenuate. I don't know if anybody's ever proven that, but it's a feature of the random medium that induces the attenuation. The periodic medium that you are concerned with acts as a certain filter. There are some questions regarding whether you have a random medium or a periodic medium. If you go to low frequencies, to what extent can you expect the effective behavior predicted to match up to the effective behavior observed? By that, I mean that you have a situation which is more random than it is periodic. It is not clear that the periodic situation in that limit adequately describes the effective behavior predicted for something which is more random-like.
- A. Nayfeh: If you use a very high frequency don't you expect to have a spread in the modes whereby you can identify the matrix by itself and the inclusion by itself?
- J.E. Gubernatis: Yes.
- A. Nayfeh: If it compares with the dimension of the inclusion, then you can see both materials.
- J.E. Gubernatis: At high frequency, the wavelength is small. I would then think that if you would go to a situation where you're replacing the wave by a ray, it has only a certain probability of intersecting a certain type of material. Now, in the case that we have here, we have a material host and a pore. We haven't considered the case where we would have two phases of materials doing the scattering.
- G.S. Kino: (Stanford University): There's a great deal of literature on this very subject. For instance, Lifshitz and Parkonovski is the standard one that everybody refers to and they've all come out with simple laws at the low frequency end and then, in my opinion, a rather suspect law as they get up in frequency. Evans and I and several other people have done a paper about five years ago on this

very subject. In ceramics where we looked at the scattered power, we did it for the use of the exact solution for the pores, and put in the distribution. You get something that looks rather like the cross-section of the scatterer, averaged over all of the distribution, essentially, so it rises and flattens off. All these curves seem to come up and flatten out. It is terribly difficult to reconcile that with the perturbation theories. A number of people have tried to do this. Again, the results are sort of suspicious. Does yours agree with these?

J.E. Gubernatis: This is one of the things which we are really attempting to test. Our curve doesn't flatten off because of the way we plotted it.

G.S. Kino: Yes, I realize that. Why did you plot it that way?

J.E. Gubernatis: Because I saw that all the curves were about the same. It just sort of struck me that this made a little bit more sense to me. On the one hand, we wanted a dimensionless parameter, so α has units of inverse length. K_0 has units of inverse length, so that was natural. But then when I did that and looked at the numbers, it struck me that there was something else there, and I divided by C and I got that. That is something that happened. What you're saying is that there are some very simple formulas which people have used which try to predict how the attenuation will behave in certain limiting regimes. The experiment doesn't always exhibit that particular behavior, but the nature of the approximations, to the extent I understand them, basically assume that all the scattered regions are independent. One of the attempts here was simply to take that particular approximation and see what's in there. What does it really truly predict? And you don't see these laws coming out. Now, relative to what you did with Evans, et al., I want to actually address those kinds of questions, and explore the fact that it seems that the extreme sizes of the particles are the controlling feature in determining attenuation.