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SHEAR WAVES IN POLYCRYSTALLINE MEDIA AND MODIFICATIONS OF THE KELLER APPROXIMATION

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Abstract—A simple closed-form solution is derived for shear waves of an arbitrary frequency in polycrystalline media by invoking the Kramers–Kronig relations. Then modifications of the Keller approximation are considered from the viewpoint of causality of the coherent wave.

INTRODUCTION

Recently Stanke and Kino[1] have presented a unified theory of elastic waves dispersion in polycrystalline materials as well as a comprehensive survey of relevant references. Unlike previous investigations their theory applies for the entire frequency interval, $0 \leqslant \omega < \infty$. Making use of the Keller approximation the authors arrive at a nonlinear equation which can be solved numerically for the phase velocity, $c(\omega)$, and the attenuation $\alpha(\omega)$.

Their theory unexpectedly shows the qualitatively different dispersive behavior of the overall longitudinal and overall shear waves in polycrystals. On introducing the limits

$$\lim_{\omega \to 0} c(\omega) = c_0, \qquad \lim_{\omega \to 0} c(\omega) = c_\infty \tag{1}$$

their results indicate that for P-mode

$$c_\infty > c_0 \tag{2}$$

while for S-mode

$$c_\infty < c_0. \tag{3}$$

No reasoning for this different behavior has been given.

We first present an alternative solution to the problem of shear wave propagation by making use of the approximate method given previously for P-waves by Beltzer and Brauner[2]. Our approach, like that of Stanke and Kino, provides $c(\omega)$ and $\alpha(\omega)$ for the entire frequency interval, but is in an extremely simple analytical form convenient for prompt evaluations. The results obtained indicate that the dispersion of shear waves is similar to that of longitudinal waves in disagreement with inequality (3).

Then we turn to the analysis of the Keller approximation and show that the reason for discrepancy lies in the non-uniqueness of this technique. By imposing the constraint of causality (see Beltzer[3]) we construct a modified version of the Keller approximation, which provides results in accord with our previous method.

GENERALIZATION OF ROKHLIN'S MODEL

A polycrystalline material consists of randomly oriented grains, which scatter elastic waves. This gives rise to the attenuation and, in turn, to the modified wave velocity. The overall dynamic response of such materials is a particular case of a general problem of wave propagation in random media. It has been shown (see for example, Lax[4], Keller[5]) that the constructive interference of scattered waves may lead to formation of a coherent wave, which describes the overall dynamic response of the medium for the entire frequency interval, $0 \leqslant \omega < \infty$.

In considering the phenomenon at hand one should note that the resort to an exact analysis seems unreasonable in view of the stochastic nature of the problem. In fact, all the known methods are essentially approximate, as well as the approach given herein.

The wave number of the coherent wave, $\tilde{k}$ is given by

$$\tilde{k} = \omega/c(\omega) + i\alpha(\omega) \tag{4}$$

where the phase velocity, $c(\omega)$ and the attenuation, $\alpha(\omega)$, depend on the microstructure. It is well established and widely accepted[1] that the attenuation, $\alpha(\omega)$, shows a pattern of behavior common for both P- and S-modes. On letting λ be the wavelength and d a typical grain size, the pattern is described as follows

$$\alpha(\omega) \sim 0(\omega^4), \qquad \text{as} \quad \lambda/d \to \infty \tag{5a}$$

$$\alpha(\omega) \sim 0(\omega^2), \qquad \text{as} \quad \lambda/d \sim 0(1) \tag{5b}$$

$$\alpha(\omega) \sim \text{constant}, \qquad \text{as} \quad \lambda/d \to 0. \tag{5c}$$

Making use of this fact and in the spirit of approximate methods, we first seek for a proper expression for $\alpha(\omega)$, which would satisfy eqns (5)[2]. Modeling a medium as an array of isotropic cells and making additional assumptions Rokhlin[6] considered the case of P-waves. He derived a simple analytical expression for $\alpha(\omega)$ which remarkably satisfies eqns (5) but provides a rather poor quantitative agreement with more refined theories. Also, no expression for $c(\omega)$ has been given. In the work of Beltzer and Brauner[2], his approach has been improved in two ways; first, by redefining the coefficients appearing in his expression for $\alpha(\omega)$ so as to achieve a better quantitative description, and, second, by determining $c(\omega)$. This method will be applied for shear waves in the rest of this section.

On adapting the functional form of Rokhlin's equation we stipulate

$$\alpha(\omega) = A(\delta\omega - \sin\delta\omega)(\gamma\omega - \sin\gamma\omega)/(\gamma\delta\omega^2) \tag{6}$$

where the coefficients A, δ, and γ are yet unspecified. The Rayleigh, stochastic and geometric asymptotes of eqn (6) are

$$\alpha(\omega) = A\delta^2\gamma^2\omega^4/36, \qquad \text{as} \quad \gamma\omega < \delta\omega < 1 \tag{7a}$$

$$\alpha(\omega) = A\gamma^2\omega^2/6, \qquad \text{as} \quad \delta\omega > 1, \gamma\omega < 1 \tag{7b}$$

$$\alpha(\omega) = A, \qquad \text{as} \quad \delta\omega > \gamma\omega > 1 \tag{7c}$$

and thus upon a proper specification of A, δ and γ, eqn (6) will satisfy eqns (5).

To this end we restrict our analysis to the case of the grains of cubic symmetry and match eqns (7) with the asymptotic values given in Stanke and Kino[1] to obtain for the case of shear waves

$$A = 1/d \tag{8a}$$

$$\delta = \{9[3+2(c_s/c_p)^5]/5\}^{1/2} d/c_s \tag{8b}$$

$$\gamma = \sqrt{\left(\frac{1}{50}\right)}(v/C_{44}^0)d/c_s \tag{8c}$$

where C_{44}^0 is the elastic Voight average, c_p and c_s are the average dilational and shear wave velocities and the anisotropy factor, ν, is

$$\nu = C_{11} - C_{12} - 2C_{44}. \tag{9}$$

Here C_{ij} are the elastic constants of a single crystal. It is supposed that δ and γ defined by eqns (8b) and (8c) comply with the inequality $\delta > \gamma$, following from eqns (7).

As far as shear waves in an effective homogeneous medium are concerned, the analysis can be confined to the case of antiplane strain, for which the coherent wave, say $\langle u_z \rangle$, can be written as

$$\langle u_z \rangle \simeq e^{-\alpha(\omega)x} e^{i\omega[x/c(\omega) - t]} \tag{10}$$

where z and x are Cartesian coordinates.

Having evaluated the attenuation, $\alpha(\omega)$, we turn to the Kramers–Kronig (K–K) relations, to find the wave velocity, $c(\omega)$[2, 7]. In fact, the coherent wave is meaningless as an overall dynamic response, unless it is causal, which implies the following K–K relation

$$c(\omega) = c_0 \left[1 + \frac{2c_0\omega^2}{\pi} \fint_0^\infty \frac{\alpha(\omega')\,d\omega'}{\omega'^2(\omega'^2 - \omega^2)} \right]^{-1} \tag{11}$$

where a slash denotes Caushy principal value. The static limit, c_0, may be derived from an independent static analysis (see, for example, [8]).

On substituting eqn (6) in eqn (11) the singular integral can be straightforwardly evaluated in a complex plane, with the poles at $\omega' = 0$, $\omega' = \pm\omega$. Note that, according to eqns (7), $\delta > \gamma$, which implies integration in the upper half-plane, as shown in Fig. 1, ($\omega = a$). Consequently, the result of integration is not interchangeable with respect to δ and γ, unlike eqn (6). In fact, the inequality $\delta > \gamma$ reflects the presence of two scales, which affect the phase velocity in different ways.

The final expression for $c(\omega)$ is

$$c(\omega) = c_0\{1 + (c_0/d)[-\cos(\delta\omega)/(\delta\omega^2) - \cos(\gamma\omega)/(\gamma\omega^2) + \sin(\gamma\omega)\cos(\delta\omega)/(\delta\gamma\omega^3) + 1/(\gamma\omega^2) - \gamma/2 + \gamma^2/(6\delta)]\}^{-1}. \tag{12}$$

Equations (6) and (12) with A, δ, and γ defined by eqns (8) represent a simple closed-form solution for harmonic causal S-waves.

For $\omega \to \infty$, eqn (12) yields the geometric limit, c_∞, as follows:

$$c_\infty = c_0[1 + (c_0/d)(-\gamma/2 + \gamma^2/6\delta)]^{-1}. \tag{13}$$

Since $\delta > \gamma$, this implies

$$c_\infty > c_0. \tag{14}$$

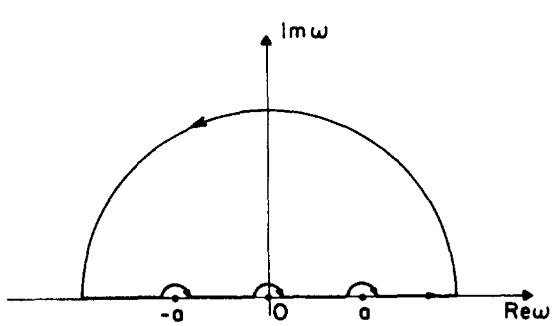

Fig. 1. Integration in a complex plane.

Table 1.

Material	c_p (km/s)	c_s (km/s)	c_0 (km/s)	$\nu \cdot 10^{11}$(N/m^2)
Fe	5.900	3.230	3.099	−1.36
Al	6.319	3.130	3.123	−0.11

In order to appreciate the physical meaning of the geometric limit, $\omega \to \infty$, it is useful to invoke the formal analogy between the coherent wave in a random elastic medium and a viscoelastic wave in a homogeneous medium. It then becomes clear that this limit describes in fact the propagation velocity of a shock (see Appendix for details). Thus, c_∞ yields the velocity of a progressing discontinuity in a polycrystalline medium provided that this preserves its linear behavior.

In the case of P-mode the above method[2] predicts the response in accord with that of Stanke and Kino. In order to compare the results for the case of S-mode, eqns (6), (8) and (12) have been applied to the materials described in Table 1. Here use has been made of the unified theory of Stanke and Kino[1] to evaluate c_0.

Figures 2 and 3 show reasonable agreement between the present theory (solid lines) and the theory of Stanke and Kino (broken lines) for the attenuation, $\alpha(\omega)$, particularly in view of the simplicity of the present model. On the other hand, Figs 4 and 5 reveal qualitatively different results for the phase velocity, $c(\omega)$. (The meaning of the dotted lines in Figs 4 and 5 will be explained in the sequel.) In view of eqn (11), which expresses $c(\omega)$ in terms of $\alpha(\omega)$ for any causal motion, the data for $c(\omega)$ presented by the broken lines appear inconsistent with the K–K relations. In fact the solutions given by these lines violate inequality (14), which is of a quite general nature and is independent of the wave mode. It is of interest that while available experiments (for example, with photoelastic materials) are insufficient for making numerical evaluations, they show an increase in the dynamic stiffness compared with the static one, in agreement with inequality (14). A particularly strong effect on Young's modulus was reported in [9] while Poisson's ratio preserved a constant value. This implies that the dynamic Lame moduli, λ and μ, may show a similar dependence on frequency in agreement with our analysis.

The reasons for the above discrepancy for $c(\omega)$ can be appreciated by considering some

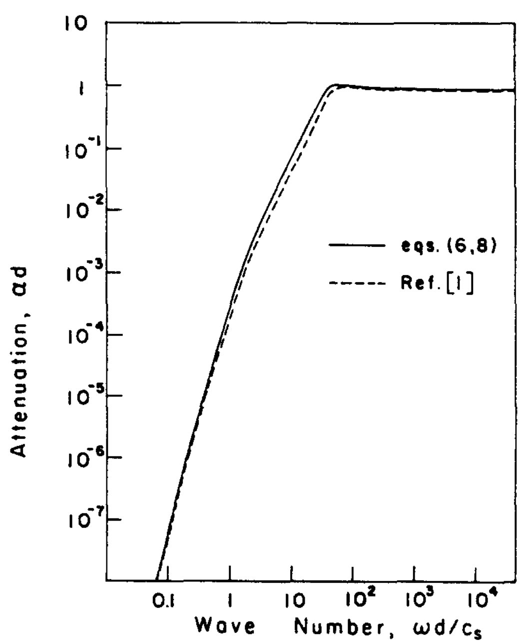

Fig. 2. Attenuation in polycrystalline aluminum.

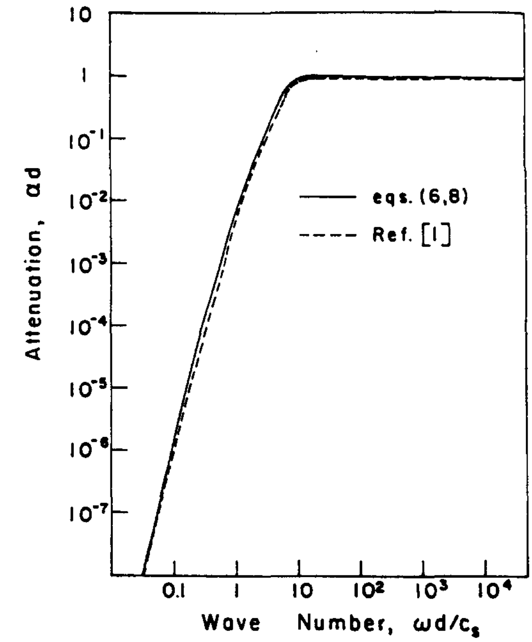

Fig. 3. Attenuation in polycrystalline iron.

of the features of the Keller approximation, applied by Stanke and Kino, which is carried out in the next section.

MODIFICATIONS OF THE KELLER APPROXIMATION

Provided that the effective homogeneous medium does exist we may resort to the coherent SH-mode, which may be thought of as arising from averaging the random

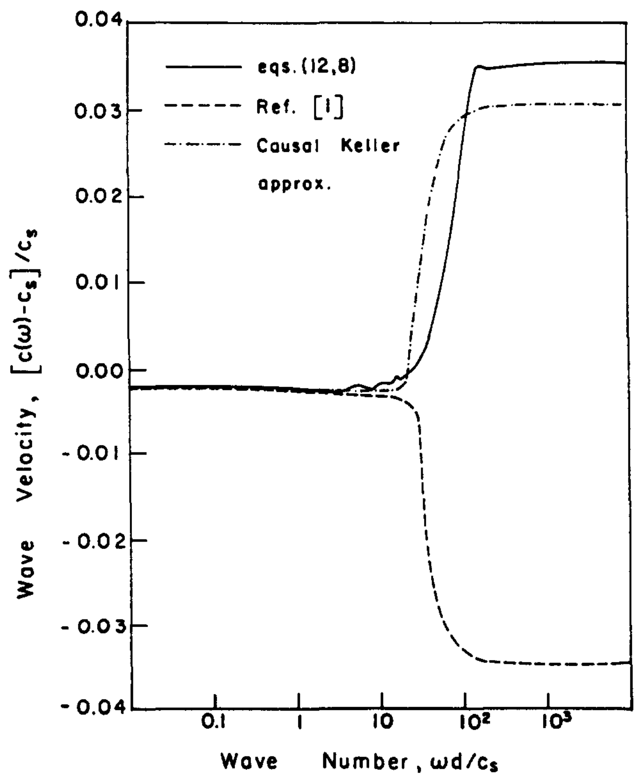

Fig. 4. Wave velocity in polycrystalline aluminum.

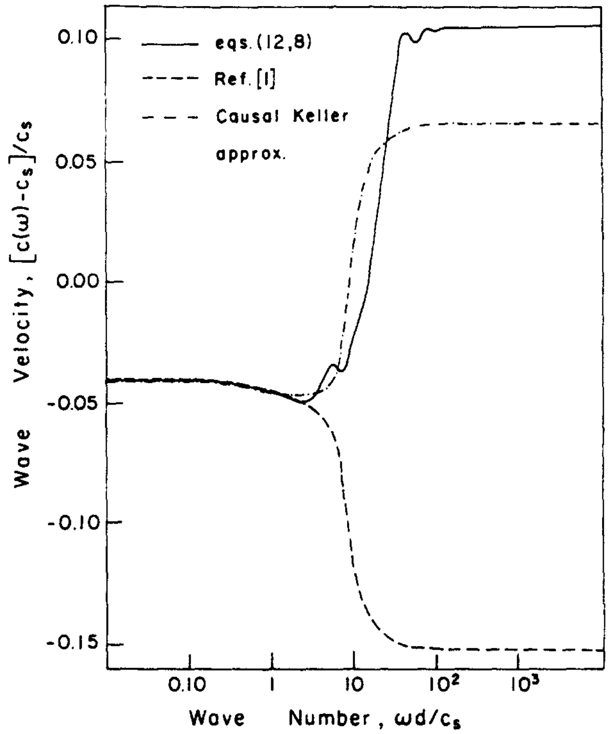

Fig. 5. Wave velocity in polycrystalline iron.

Helmholtz equation. For the case of the correlation function, $W(r)$,

$$W(r) = e^{-r/a} \tag{15}$$

with $a = d/2$, the Keller approximation provides[10]†

$$\tilde{q}^2 = q_0^2 + \varepsilon^2 q_0^2 - 2i\varepsilon^2 q_0^4[(a^{-1} - iq_0 - i\tilde{q})^{-1} - (a^{-1} - iq_0 + i\tilde{q})^{-1}]/\tilde{q} \tag{16}$$

with

$$\tilde{q} = \tilde{k}a, \tag{17}$$

and $q_0 = k_0 a$ being the average wave number and ε the inhomogeneity parameter. Focusing on a mainly qualitative analysis we consider in what follows the solutions of this equation, which is much simpler than the more accurate but cumbersome eqn (102) of Stanke and Kino[1]. Numerical results provided by eqn (16) are close to those following from the electromagnetic analogy investigated in the above work, at least within the accuracy of the graphical data presented on a logarithmic scale.

At low frequency eqn (16) has the solution

$$(q/q_0)^2 \approx 1 + \varepsilon^2[1 - (i2q_0)^2]/(1 - i2q_0) \tag{18}$$

whereas for the geometric limit, when $q_0 \gg 1/\varepsilon$, it yields

$$(q/q_0) \approx 1 \mp \varepsilon + i/2q_0. \tag{19}$$

Since the Keller approximation does not provide a unique solution, physical considerations must play the major role in its applications. In fact, eqn (16) has generally four

† In eqn (16) the correlation coefficient $\langle \mu^2 \rangle$ has been taken as unity.

solutions, two of which should be put aside as providing $\alpha(\omega) < 0$, which is inadmissible. Confining our analysis to the case of iron, $\varepsilon = 0.135$[1], for which the effect of interest is more explicit than for aluminum, we show the remaining two solutions in Fig. 6.

Next, the attenuation corresponding to the upper branch (the broken line, Fig. 6(a)) clearly violates eqn (5a) at low frequencies. Accordingly, the conclusion may be drawn that this is the lower branch which provides the solution for the entire interval, $0 \leqslant \omega < \infty$ (the solid line, Figs 6(a) and (b)). However this branch, given by eqn (18) at low frequency and by eqn (19) (with positive perturbation term) at high frequency, violates the inequality (14).

A way of constructing a physically meaningful solution in the framework of the Keller approximation is thus to pass from the lower branch to the upper one somewhere in the range of intermediate frequencies, $1 < k_0 a < 10$. Fortunately, the gap in this interval is quite small and the "jump" appears consistent with the approximate nature of the whole method.

Another possibility is to use the Keller approximation jointly with the K–K relations. In the framework of this approach, we adopt the attenuation $\alpha(\omega)$, associated with the lower branch, making use of the basic fact that it satisfies eqns (5). Then, this expression

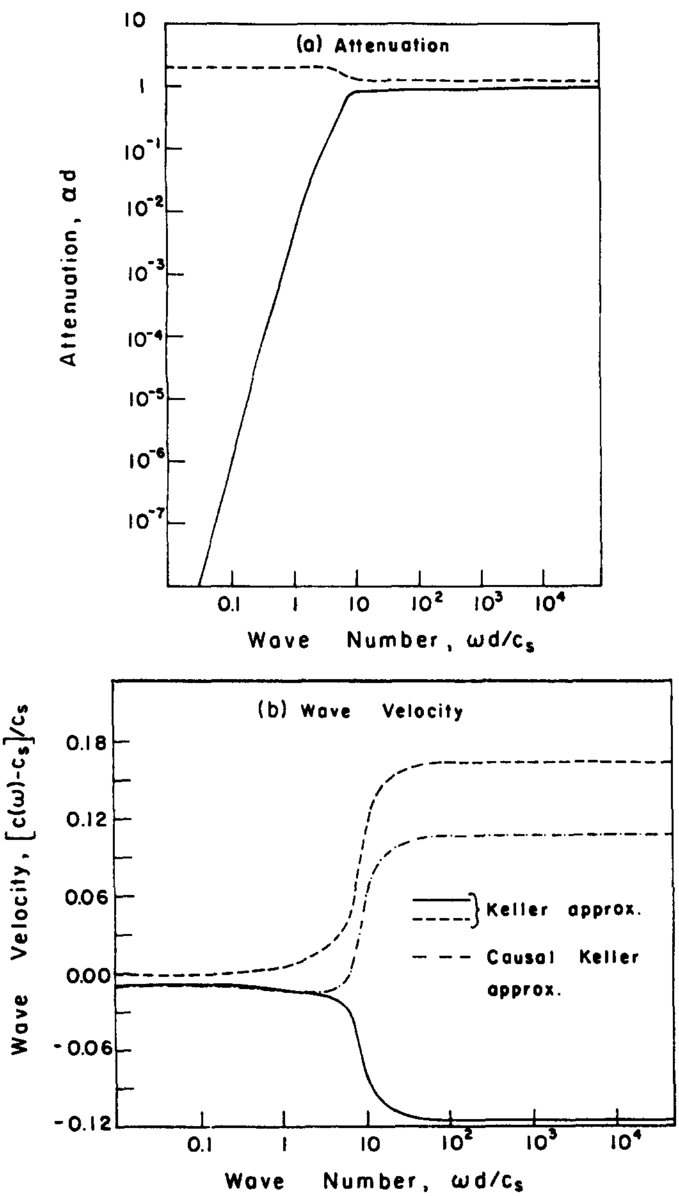

Fig. 6. Attenuation and wave velocity in polycrystalline iron via the Keller approximations.

can be substituted into eqn (11) to evaluate the phase velocity. This results in $c(\omega)$, which is close to the lower branch at low frequency and to the upper one at high frequency, as shown in Fig. 6(b) by the dotted line. Moreover, following this way, we can adopt the best known value of c_0, which may not be necessarily the one provided by eqn (16). This approach might be referred to as the causal Keller approximation.

Now we may return to Figs 4 and 5. It appears that the algorithm of the numerical solution represented by the broken lines, has not included a passage to the upper branch and followed exclusively the lower one. In fact, if we apply the causal Keller approximation (CKA) described above, and adopt c_0 from the unified theory of Stanke and Kino, we arrive at the results shown by the dotted lines, which are in agreement with the solution obtained in the previous section (solid lines). The advantage of the CKA is thus a capability of providing a unique causal solution for the entire frequency interval.

CONCLUSIONS

A simple closed form solution to shear waves of an arbitrary frequency in polycrystalline media has been derived by generalizing Rokhlin's model. It has been shown that the transition from one branch to another may be necessary in the context of the Keller approximation to arrive at a response consistent with causality of the coherent wave. An alternative way is to use the causal Keller approximation which incorporates the Kramers–Kronig relations. Applications of this approach to more complicated models, such as the one proposed by Stanke and Kino, would be of interest.

It should be noted that the results presented hold under the basic concept of an effective homogeneous medium which is capable of supporting plane waves of the type given by eqn (10).

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APPENDIX

The analogy between elastic coherent waves in random media and viscoelastic waves in homogeneous media

Here we present in a condensed way some of the results given by Beltzer[11].

Despite the completely different physical mechanisms the formal analogy indicated in the title of the Appendix takes place in the sense that the frequency-dependent functions, $\alpha(\omega)$ and $c(\omega)$, say nothing about the actual mechanism of dispersion, which may be of either viscoelastic or incoherent nature. In fact, eqn (4) closely resembles a viscoelastic wave. Moreover, limiting values of $\tilde{k}$ for small and large frequencies usually conform with the conditions formulated in the theory of viscoelasticity[12]. This analogy has been used in particular cases by Sve[13] and Cowin[14] and can be further appreciated by the following consideration.

We introduce the constitutive law

$$\langle \tau \rangle = \tilde{E} \langle \varepsilon \rangle \tag{A.1}$$

where $\langle \tau \rangle$ is the average (coherent) stress, and $\langle \varepsilon \rangle$ the average strain associated with coherent displacements in a usual manner. These values vary harmonically in time. The modulus, $\tilde{E}$, is then complex-valued and frequency dependent and is given by

$$\tilde{E} = \tilde{c}^2 \rho_0 \tag{A.2}$$

where ρ_0 is the average density and $\tilde{c}$ is the complex velocity defined in terms of $c(\omega)$ and $\alpha(\omega)$ as follows:

$$\text{Re } \tilde{c} = c\omega^2/(\omega^2 + \alpha^2 c^2) \tag{A.3}$$

$$\text{Im } \tilde{c} = -\alpha\omega c^2/(\omega^2 + \alpha^2 c^2). \tag{A.4}$$

Then,

$$\text{Re } \tilde{E}(\omega \to \infty) = c_\infty^2 \rho_0, \quad \text{Im } \tilde{E}(\omega \to \infty) = 0, \quad \text{Re } \tilde{E}(\omega = 0) = c_0^2 \rho_0, \quad \text{Im } \tilde{E}(\omega = 0) = 0.$$

Now it can be shown[12] that a discontinuity wave in a linear medium governed by eqn (A.1) propagates with the velocity of the geometric limit, c_∞.