LA-UR-84-2741

CONF-840738--2

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LA-UR--84-2741

DE84 016773

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SUBMITTED TO The proceedings of the meeting, "Review of Progress in Quantitative NDE" at the University of California-San Diego, La Jolla, CA 7/8-13/84.

ELASTIC WAVE PROPAGATION THROUGH POLYCRYSTALS

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INTRODUCTION

Propagating elastic waves are commonly used to characterize nondestructively polycrystalline microstructure. To develop a fully quantitative characterization procedure, one needs a better understanding of what microstructural features most strongly influence the propagation and how these features appear in the measured, frequency dependent, wave speed and attenuation. We report on our progress in a first principle investigation of these questions. We started with the equations of motion for elastic wave propagation and systematically developed a new approximation that is both well characterized and a potential improvement upon existing approximations. One of our objectives is studying the sensitivity of this approximation to changes in microstructural parameterization.

The seminal work for existing approximations was done by Lifshits and Parkhomovskii.[1] They characterized the crystallite to crystallite variations in elastic stiffness by a field $\Delta C_{ijkl}(\vec{r})$, which was measured relative to an average material, and derived expressions for effective wave speed and attenuation for crystallites with cubic symmetry to second order in ΔC_{ijkl}. After making the effective medium approximation, that is, assuming the average displacement field was a constant amplitude plane wave, they asymptotically evaluated these expressions at high and low frequencies. Microstructural details, to the level of approximation considered, became embodied in a correlation function $W(\vec{r}-\vec{r}')$ that gives the probability of $\vec{r}$ and $\vec{r}'$ being in the same crystallite.

Recently, Kino and Stanke[2] extended the Lifshits-Parkhomovskii work. As Lifshits-Parkhomovskii, they developed an effective medium approximation to the wave equation, but by adapting an approximation of Karal and Keller[3] and evaluating the necessary integrals and configurational averages exactly, they produced an approximation for the wave speed and attenuation for which the Lifshits-Parkhomovskii theory is an approximation and the a priori restriction to use at high and low frequencies was removed. An additional aspect of the Kino-Stanke work was the experimental determination that $W(r)$ appears well approximated by $\exp(-r/L)$. This form simplifies the evaluation of the required spatial integrations and embodies all microstructural information into a single parameter L.

Our work advances in the direction developed by Lifshits-Parkhomovskii and Kino-Stanke, but with several important differences: Our resulting equations are not restricted to crystallites of cubic symmetry. We performed the necessary orientational averages analytically and generally (triclinic crystallites). Also, our approximation is not second order in $\Delta C_{ijkl}(\vec{r})$. In the perturbation series for the average displacement field, we selectively summed an infinite series of terms in products of $\langle \Delta C_{ijkl} \Delta C_{mnpq} \rangle$ to produce and approximation of infinite order in the anisotropy. Additionally, we did not have to make the effective medium approximation. We are in a position to test its consequences.

In this report we restrict ourselves to summarizing the basic nature of our approximation, contrasting it with those of Lifshits-Parkhomovskii and Kino-Stanke, and highlighting the important differences from a perturbation-theoretic point of view.

AVERAGE FIELDS

Our starting point is the equation of motion for the steady-state, displacement field Green's tensor of an elastic medium in which the elastic stiffness varies from point to point[4]

$$\frac{\partial}{\partial x_j} C_{ijkl}(\vec{r}) \frac{\partial}{\partial x_l} G_{im}(\vec{r},\vec{r}') + \rho\omega^2 G_{im} + \delta_{im}\, \delta(\vec{r}-\vec{r}') = 0 \tag{1}$$

After defining $C_{ijkl}(\vec{r}) = C^o_{ijkl} + \Delta C_{ijkl}(\vec{r})$, where C^o_{ijkl} is a constant tensor taken to be $\langle C_{ijkl} \rangle$, we can convert (1) into an equivalent integral equation that for present purposes is most conveniently expressed in terms of the Fourier transforms of the physical quantities of interest. Symbolically, we write this equation as

$$G = G^o + G^o V G \tag{2}$$

where

$$G_{ij}(\vec{k},\vec{q}) = \frac{1}{(2\pi)^3} \int d\vec{r} \int d\vec{r}'\, G_{ij}(\vec{r},\vec{r}')\, e^{-i\vec{k}\cdot\vec{r}}\, e^{i\vec{q}\cdot\vec{r}'} \tag{3a}$$

$$G^o_{ij}(\vec{k},\vec{q}) = G^o_{ij}(\vec{k})\,\delta(\vec{k}-\vec{q})$$

$$= \frac{1}{4\pi\rho\omega^2} \left[\frac{\hat{k}_i \hat{k}_j}{k^2-\alpha_0^2} + \frac{\delta_{ij}-\hat{k}_i \hat{k}_j}{k^2-\beta_0^2} \right] \delta(\vec{k}-\vec{q}) \tag{3b}$$

and

$$V_{ij}(\vec{k},\vec{q}) = k_m \Delta C_{imjn} q_n \qquad (3c)$$

with ρ being the crystallite density, ω the angular frequency, α_0 the longitudinal wavenumber associated with C^{o}_{ijkl}, and β_0 the transverse wavenumber.

From (2) we seek to determine the poles of $\langle G \rangle$. From the real part of these poles, we obtain the phase velocity of the average wave; from the imaginary parts, the attenuation. To proceed we make the ansatz that

$$\langle G_{ij}(\vec{k},\vec{q})\rangle = G_{ij}(\vec{k})\ \delta(\vec{k}-\vec{q}) \qquad (4)$$

which is simply a statement that the averaging restores translational invariance to the material. In the effective medium approximation this same ansatz is made along with the assumption that $\langle G_{ij}(\vec{k},\vec{q})\rangle$ has the same form as $G^{o}_{ij}(\vec{k})$; that is, (4) is given by right-hand side of (3b) with α_0 and β_0 replaced by the to be determined α and β. We are, however, able to show that

$$G_{ij}(k) = G_l(k)\hat{k}_i\hat{k}_j + G_t(k)(\delta_{ij}-\hat{k}_i\hat{k}_j)$$

where

$$G_l(k) = \frac{1}{k^2 - \alpha_0^2 - M_l(k)}$$

$$G_t(k) = \frac{1}{k^2 - \beta_0^2 - M_t(k)}$$

which implies a pole structure different and potentially more complicated than allowed by the effective medium approximation. The M_l and M_t are the longitudinal and transverse parts of a quantity we call the average proper self-energy, terminology developed in quantum field theory. This self-energy appears in the integral equation for $\langle G \rangle$; that is, we can show[5]

$$\langle G \rangle = G^0 + G^0 \langle M \rangle \langle G \rangle \qquad (5)$$

and that

$$M = V + M\langle G \rangle (V - \langle M \rangle) \qquad (6)$$

These equations represent an exact solution to the problem. Since $\langle G \rangle$ depends on M, and M depends on $\langle G \rangle$, they are coupled nonlinear, integral equations. The advantage of expressing the solution in this form is the potential for a systematic development of perturbation theory, particularly perturbation theory to infinite order in V.

To derive (5) and (6) we start[5] by iterating (2)

$$G = G^o + GVG^o + G^oVG^oVG^o + \ldots$$
$$= G^o + G^o(I + VG^oV + VG^oVG^o + \ldots)G^o$$
$$= G^o + G^oTG \quad . \tag{7}$$

where the scattering operator T equals

$$T = V(I + G^oV)^{-1} \tag{8}$$

Next, we average (7) to obtain

$$\langle G\rangle = G^o + G^o\langle T\rangle G^o \tag{9}$$

and then we solve this equation for G^o

$$G^o = (I + G^o\langle T\rangle)^{-1} \langle G\rangle \tag{10}$$

Then we substitute this result for the last G^o in (9) to produce (6)

$$\langle G\rangle = G^o + G^o \langle M\rangle\langle G\rangle \tag{11}$$

where

$$\langle M\rangle = \langle T\rangle \ (I + G^o\langle T\rangle)^{-1} \tag{12}$$

To derive (6), which leads for present purposes to a more useful form for $\langle M\rangle$, we solve (11) for G^o

$$G^o = (I + \langle G\rangle\langle M\rangle)^{-1} \langle G\rangle \tag{13}$$

and substitute this result for the last G^o in (7) to convert it to

$$G = G^o + G^o \ T(I + \langle G\rangle\langle M\rangle)^{-1} \langle G\rangle$$

For the average of this equation to be consistent with (11) we must have

$$M = T(I + \langle G\rangle\langle M\rangle)^{-1}$$
$$= V(I - G^oV)^{-1} \ (I + \langle G\rangle\langle M\rangle)^{-1}$$

which upon replacement of G^o by (13) reduces straightforwardly to

$$M = V(I - \langle G\rangle(V - \langle M\rangle))^{-1}$$

or

$$M = V + M\langle G\rangle(V - \langle M\rangle)$$

the desired result.

To illustrate the connection of these results to perturbation theory, we write

$$M = M_1 + M_2 + M_3 + M_4 + \ldots$$

where the subscript denotes the order of the corresponding term in V. We find that

$$M_1 = V$$

$$M_2 = V\langle G\rangle V - V\langle G\rangle\langle V\rangle$$

$$M_3 = -V\langle G\rangle(V\langle G\rangle V - \langle V\rangle\langle G\rangle\langle V\rangle) + (V\langle G\rangle V - V\langle G\rangle\langle V\rangle)\langle G\rangle(V - \langle V\rangle)$$

When we substitute these results into the right-hand side of (6), average both sides of the resulting equations, and use the result that $\langle V\rangle = 0$, we find that

$$\langle M\rangle = \langle V\langle G\rangle V\rangle + \langle V\langle G\rangle V\langle G\rangle V\rangle + \langle V\langle G\rangle V\langle G\rangle V\langle G\rangle V\rangle - \langle V\langle G\rangle V\rangle\langle G\rangle\langle V\langle G\rangle V\rangle + O(V^5) \tag{14}$$

But $\langle G\rangle$ can, through (5) and (14), be expressed in terms of V and G^o. The resulting expression for $\langle M\rangle$ is

$$\begin{aligned}\langle M\rangle = {} & \langle VG^oV\rangle - \langle VG^oV\rangle G^o\langle VG^oV\rangle \\ & + \langle VG^o\langle VG^oV\rangle G^oV\rangle - \langle VG^oV\rangle G^o\langle VG^o\langle VG^oV\rangle G^oV\rangle \\ & - \langle VG^o\langle VG^oV\rangle G^oV\rangle G^o\langle VG^oV\rangle + \langle VG^o\langle VG^oV\rangle G^oV\rangle G^o\langle VG^o\langle VG^oV\rangle G^oV\rangle \\ & + \ldots \\ & + \langle VG^oVG^oV\rangle + \ldots\end{aligned}$$

The terms implied in the first four lines originate from the first term in (14); hence, having $\langle M\rangle$ depend on $\langle G\rangle$ and vice versa is simply a way of compactly representing such infinite series of terms. Since V represents the crystalline anisotropy, any approximation to $\langle M\rangle$ based on $\langle V\langle G\rangle V\rangle$ is thus of infinite order in the anisotropy. In the next section we adopt this approximation, discuss some of its basic features, and contrast it to the approximations of Lifshits-Parkhomovskii and Kino-Stanke

APPROXIMATIONS

The poles of $\langle G\rangle$ satisfy

$$k^2 - \alpha_o^2 - M_l(k) = 0 \tag{15a}$$

$$k^2 - \beta_o^2 - M_t(k) = 0 \tag{15b}$$

Since M_l and M_t depend on $\langle G\rangle$ and hence its poles, these equations are coupled. We will denote the solutions to these equations by α and β and signify the dependency of M on $\langle G\rangle$ by $M[\alpha,\beta]$, that is, by the location of the poles of $\langle G\rangle$. Our basic approximation is to take for $\langle M\rangle$ the leading term in (14)

$$\langle M[\alpha,\beta]\rangle \simeq \langle V\langle G[\alpha,\beta]\rangle V\rangle \tag{16a}$$

where

$$\langle G\rangle = G^o(I - \langle M\rangle G^o)^{-1} \tag{16b}$$

As discussed in the last section, these equations represent a perturbation series to infinte order in V. In particular, our approximation for $\langle G\rangle$ is

$$\begin{aligned}\langle G\rangle = {} & G^o + G^o\langle VG^oV\rangle G^o + G^o\langle VG^o\langle VG^oV\rangle G^oV\rangle G^o \\ & - G^o\langle VG^oV\rangle G^o\langle VG^oV\rangle G^o - G^o\langle VG^oV\rangle G^o\langle VG^o\langle VG^oV\rangle G^oV\rangle G^o \\ & + \ldots\end{aligned} \tag{17}$$

The Kino-Stanke approximation can be characterized by

$$\langle M[\alpha,\beta]\rangle \simeq \langle V\langle G[\alpha,\beta]\rangle V\rangle$$

$$\langle G\rangle \simeq G^o[\alpha,\beta] = G^o[\alpha_o,\beta_o](I-\langle M\rangle G^o[\alpha_o,\beta_o])^{-1}$$

These approximations lead to

$$\alpha^2 - \alpha_o^2 - m_l(\alpha) = 0 \tag{18a}$$

$$\beta^2 - \beta_o^2 - m_t(\beta) = 0 \tag{18b}$$

which are an uncoupled set of equations for α and β. If we make the effective medium approximation, our $M_l[\alpha,\beta]$ and $M_t[\alpha,\beta]$ would equal Kino-Stanke's $m_l[\alpha,\beta]$ and $m_t[\alpha,\beta]$. In terms of a perturbation series for $\langle G\rangle$, their approximation is equivalent to

$$\begin{aligned}\langle G\rangle & = G^o[\alpha,\beta] \\ & = G^o + G^o\langle VG^oV\rangle G^o + G^o\langle VG^oV\rangle G^o\langle VG^oV\rangle G^o \\ & \quad + G^o\langle VG^oV\rangle G^o\langle VG^oV\rangle G^o\langle VG^oV\rangle G^o + \ldots\end{aligned} \tag{19}$$

which of infinite order in V.

The Lifshits-Parkhomovksii approximation can be characterized by

$$\langle M[\alpha,\beta]\rangle \sim \langle VG[\alpha,\beta]V\rangle$$

$$\langle G[\alpha,\beta]\rangle \sim G^o[\alpha,\beta] = G[\alpha_o,\beta_o] + G^o[\alpha_o,\beta_o]\langle M\rangle G^o[\alpha_o,\beta_o]$$

which lead to an uncoupled set of equations for α and β.

$$\alpha^2 - \alpha_o^2 - m_l(\alpha_o) = 0 \tag{20a}$$

$$\beta^2 - \beta_0^2 - m_t(\beta_o) = 0 \tag{20b}$$

In terms of a perturbation series for $\langle G\rangle$ their approximation is simply

$$\langle G\rangle = G^o + G^o\langle VG^oV\rangle G^o \tag{21}$$

REMARKS

In the absence of any effective medium approximation, (21), (19), and (17) represent a clear heirarchy in level of approximation. How significant is the effect of the effective medium approximation is at this time unknown. We do know, however, that our approximation (17) is formally equivalent to Kraichnan's direct interaction approximation[6] (the DIA) developed for wave propagation in turbulent medium. Using a $W(r) \sim \exp(-r/L)$, Frisch[7] shows for scalar waves that the effective medium approximation to the DIA is very good. If this same fidelity is true for the elastic wave problem, then (17) with the effective medium approximation will reduce to a set of equations just slightly more complicated than those of Kino and Stanke. Objectives of computations under way include studying the utility of the effective medium approximation and the quanitative difference between (17) and (19). The results of these computations, as well the details of our analytic methods, will be reported elsewhere.

ACKNOWLEDGEMENTS

This work was supported by the Department of Energy. One of us (AAM) thanks the Center for Materials Science of the Los Alamos National Laboratory for their hospitality during the course of the work.

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