PROPAGATION OF ELASTIC WAVES IN EQUIAXED IRON POLYCRYSTALS
WITH ALIGNED [001] AXES

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INTRODUCTION

A polycrystalline material is composed of numerous discrete grains, each having a regular, crystalline atomic structure. The elastic properties of the grains are anisotropic and their crystallographic axes are differently oriented. Thus the anisotropic nature of elastic wave propagation in a number of structural materials, such as austenitic stainless steel welds and castings, used in nuclear power plants stems from the details of their grain structures. Columnar grain structure is seen in the austenitic stainless steel welds while the microstructure of cast stainless could vary from randomly oriented equiaxed grains to highly oriented columnar grains. An acoustic wave travelling through such a microscopically inhomogeneous medium suffers scattering and consequently has frequency dependent attenuation and phase velocity that depend on the grain structure. This paper is motivated by the desire to better understand these effects.

Figure 1 shows typical microstructures of austenitic stainless steel weld metal and centrifugally cast stainless steel [1]. Both microstructures reveal the presence of highly oriented columnar grains leading to a macroscopically textured medium. A lack of the knowledge of the presence of elastic anisotropy due to these favored grain orientations can create problems in ultrasonic nondestructive testing. Consequently, an effort has been undertaken in the present work to understand the behaviour of effective wave propagation constants in this kind of textured materials.

This paper presents a theory for elastic wave propagation in polycrystals of cubic crystallite symmetry with the aforementioned texture in which the [001] crystallographic axes of all grains are parallel to the z-axis of the laboratory coordinate system. The remaining crystallographic axes [100] and [010] are randomly oriented leading to a transversely isotropic material. The second-order unified theory of Stanke and Kino [2], which is valid when the single crystal anisotropy is not large, has been extended to arrive at the present theory. To this order of approximation, some degree of multiple scattering by individual grains is accounted for. In order to simplify the associated algebra, the highly oriented columnar grains have been
replaced with highly oriented equiaxed grains. Numerical results for both longitudinal and shear waves in this model material were calculated and compared with other existing theories. The material properties of this idealized medium were chosen to be the same as those of austenitic weld metal type 304 [3].

THEORY

Formal Approach

The displacement field associated with the propagation of an elastic wave through a polycrystalline material is governed by the stochastic wave equation

\[
\left[ C_{ijkl}^{\xi} \left( \vec{r} \right) u_{k,il}^{\xi} \left( \vec{r} \right) \right]_j + \rho \omega^2 u_{i}^{\xi} \left( \vec{r} \right) = 0,
\]

where \( \xi \) represents a particular medium of an ensemble of possible media \( \Xi \), \( u_{i}^{\xi} \left( \vec{r} \right) \) is the actual field in the medium \( \xi \), and the notation \( \partial_j \) denotes differentiation. We define the perturbation of the local elastic tensor \( C_{ijkl}^{\xi} \left( \vec{r} \right) \) from the isotropic homogeneous elastic tensor as

\[
\epsilon \Delta_{ijkl}^{\xi} \left( \vec{r} \right) = C_{ijkl}^{\xi} \left( \vec{r} \right) - C_{ijkl}^{\xi},
\]

where \( C_{ijkl}^{\xi} \) is the unweighted Voigt averaged elastic tensor. Our goal is to find the expected propagation constants from the expected properties of the media. Application of the second-order Keller approximation [4] to equations (1) and (2) yields the equation for the expected displacement field,
\[ 0 = C_{ijkl}(u_k^t(\vec{r}))_{ijl} + \rho \omega^2(u_i^t(\vec{r})) + \epsilon \left\{ \langle \Delta_{ijkl}(\vec{r}) \rangle \langle u_k^t(\vec{r}) \rangle \right\}_{ijl} \]

\[-\epsilon^2 \left\{ \langle \Delta_{ijkl}(\vec{r}) \rangle \int_G G_{km,l}(\vec{r} - \vec{r'}) \left[ \Delta_{mnpq}^{ijl}(\vec{r'}) \langle u_p^t(\vec{r'}) \rangle \right]_{n'n'} \, dv' \right\}_{ijl} \]

\[+ \epsilon^2 \left\{ \langle \Delta_{ijkl}(\vec{r}) \rangle \int_G G_{km,l}(\vec{r} - \vec{r'}) \left[ \Delta_{mnpq}^{ijl}(\vec{r'}) \langle u_p^t(\vec{r'}) \rangle \right]_{n'n'} \, dv' \right\}_{ijl}. \]

The angled brackets in equation (3) represent the ensemble averages. The Green's function \( G_{km} \) used above has been taken from the work of Lifshits and Parkhamovski [5].

In order to simplify the averages, we will assume that the media are statistically homogeneous, i.e., the ensemble averages are independent of position. The only property of the media which affects the one-point average \( \langle \Delta_{ijkl}(\vec{r}) \rangle \) is the rotation of the crystallographic axes of the grain containing \( \vec{r} \) with respect to the laboratory coordinate system. In addition, following Stanke and Kino [2], we also assume that the Euler angles of the grains in the ensemble are statistically independent. Then for plane waves propagating in the \( \hat{z} \) direction,

\[ u_i(\vec{r}) = a \hat{u}_i e^{-ikr \hat{z}}, \]  

equation (3) simplifies to the following equation for the expected propagation constant \( k \) for arbitrary crystallite symmetry with macroscopic texture.

\[ 0 = \left( C_{ijkl} + \epsilon \langle \Delta_{ijkl} \rangle \right) \hat{u}_k \hat{z}_j \hat{z}_i - \frac{\omega^2}{k^2} \hat{u}_i \]

\[-\epsilon^2 \left[ \langle \Delta_{ijkl} \Delta_{mnpq} \rangle - \langle \Delta_{ijkl} \rangle \langle \Delta_{mnpq} \rangle \right] \]

\[\times \int_G G_{km}(\vec{s}) \left[ W(\vec{s}) e^{ik\hat{z}\hat{z}} \right]_{n'n'} \hat{u}_p \hat{z}_j \hat{z}_q \, dv. \]

Here \( W(\vec{s}) \), which represents the geometric autocorrelation function, appears during the process of evaluating the two-point average in equation (3). Physically, this term represents the probability that two points separated by \( \vec{s} \) are in the same grain.

**Particular Case for Calculations**

We have carried out calculations for polycrystals of cubic symmetry where the grains are assumed to be equiaxed. This assumption enables us to replace \( W(\vec{s}) \) by \( W(\vec{s}) \) which greatly simplifies the evaluation of Green's integral in equation (5). Following Stanke and Kino, the geometric autocorrelation function is assumed to have the form [2]

\[ W(\vec{s}) = e^{-2s/d}, \]  

\[ 2001 \]
where \(d\) is the mean grain diameter. As pointed out by Stanke, this choice for \(W(s)\) is a good model for real materials [6]. As mentioned before, the particular texture considered in this work has the [001] crystallographic axes of all grains parallel to the \(z\)-axis of the laboratory coordinate system while the [100] and [010] axes are randomly oriented. This simplifies the averaging procedure. For example

\[
(f) = \frac{1}{2\pi} \int_0^{2\pi} f(\phi) \, d\phi.
\]  

(7)

The assumption that the grains have cubic symmetry can be stated mathematically as

\[
C_{ijkl}(\vec{r}) = \lambda (\delta_{ij} \delta_{kl}) + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + 3 \alpha_i \alpha_j \alpha_k \alpha_l.
\]

(8)

where \(\lambda\) and \(\mu\) are the Lame constants in the isotropic case, i.e., when the anisotropy factor \(A\) is zero \((A = C_{11} - C_{12} - 2C_{44})\), and \(\alpha_i\) is the cosine of the angle between the \(i\)th laboratory axis and the \(p\)th crystallographic axis of the grain containing \(\vec{r}\). We have used the symbolic manipulation code Mathematica to evaluate the necessary averages and sums in equation (5). After carrying out the necessary algebra in equation (5), the expected propagation constants for \(p\)-waves in the \(y\)-direction is given by the algebraic equation

\[
\left(1 + \frac{0.15A}{C_{22}^o}\right) \chi_i^2 = \chi_{ol}^2 + \frac{\chi_{os}^2 A^2}{\chi_{ol}(C_{22}^o)^2} \left[\frac{3\chi_{os}^2(8 + \chi_{os}^2)}{128\chi_i^4} + \frac{\chi_{ol}^2}{8\chi_i^2} - \frac{3\chi_{os}^2(8 + \chi_{os}^2)}{128\chi_i^4}\right]
\]

\[
+ \frac{32(4 + \chi_i^2 - \chi_{ol}^2 + 4i\chi_{col})}{256\chi_i^4} + \frac{32(4 + \chi_i^2 - \chi_{os}^2 + 4i\chi_{os})}{256\chi_i^4} - \left\{ \frac{3}{4\chi_i^2} \right\}
\]

\[
+ \left\{ \frac{9\chi_{os}^2}{16\chi_i^2} + \frac{11\chi_{col}^2}{32\chi_i^2} + \frac{13\chi_{ol}^2}{256\chi_i^4} + \frac{9\chi_{os}^2}{64\chi_i^2} + \frac{13\chi_{ol}^2}{256\chi_i^4} + \frac{9\chi_{os}^2}{256\chi_i^4} \right\}
\]

\[
\times \tan^{-1}\left(\frac{\chi_i}{2 + i\chi_{col}}\right) + \left\{ \frac{3\chi_{os}^2}{256\chi_i^4} \right\} \tan^{-1}\left(\frac{\chi_i}{2 + i\chi_{col}}\right) - i \left\{ \frac{3(\chi_{ol} - \chi_{os})}{16} \left(\frac{1}{\chi_i^4} + \frac{1}{\chi_i^2}\right) \right\}
\]

\[
+ \frac{3(\chi_{os}^3 - \chi_{os}^3)}{32\chi_i^4} + \frac{3(\chi_{os}^5 - \chi_{os}^3)}{256\chi_i^4} - \frac{8(4 + \chi_i^2 - \chi_{os}^2 + 4i\chi_{col})}{128\chi_i^4} \right\},
\]

(9)

where \(\chi_i = k_i d\), \(\chi_{ol} = k_{ol} d\), \(\chi_{os} = k_{os} d\), \(k_i\) is the expected wave number for \(p\)-waves in the textured medium and \(k_{ol}\) and \(k_{os}\) are the unperturbed wave numbers for \(p\)-waves and \(s\)-waves respectively, in the homogeneous medium.

We have also arrived at a similar expression for \(s\)-waves propagating in the \(y\)-direction with polarization in the \(x\)-direction. In a textured medium, waves with arbitrary propagation direction are, in general, not purely longitudinal or shear. However, when the single crystal anisotropy is not large, the deviations of the polarizations
from those of pure modes are small. Neglecting that deviation in polarization for longitudinal wave propagation at arbitrary directions in the $y$-$z$ plane, we were also able to develop an algebraic equation for the expected propagation constants.

RESULTS AND DISCUSSIONS

To obtain the normalized attenuation coefficient $\alpha/k_o$ and the normalized shift in phase velocity $(V - V_o)/V_o$ for plane waves in the considered textured medium, the algebraic equations for the expected propagation constants were solved numerically on a digital computer. In the process, the single crystal elastic constants were chosen to be the same as those used by Hirsekorn [3]. In accordance with the notation employed here, the directions $x$ and $y$ are interchangeable.

Figure 1(a) shows the dependence of the normalized attenuation coefficient $\alpha/k_o$ on the normalized frequency $\chi_{ol}$ for $p$-waves propagating in the $y$-direction. Qualitatively, this curve has the same shape as the corresponding curve for the untextured material. There appears a strong dependence of attenuation coefficient on $\chi_{ol}$ in the Raleigh region and in the Raleigh-stochastic transition region. In other words, in these frequency regimes, the larger grains cause greater amplitude attenuation. The symbols in this figure represent the corresponding results of Hirsekorn [3]. There is a good overall agreement between the present results and those of Hirsekorn except in the transition between the Raleigh and the stochastic region where the latter shows oscillatory behaviour. These oscillations of Hirsekorn's results can be attributed to the fact that in her theory all grains were assumed to have the same size and shape [7]. Figure 1(b) shows the variation of the normalized attenuation coefficient with the angle between the propagation direction and the $z$-axis (axis of rotation symmetry) measured in the $y$-$z$ plane, with $\chi_{ol}$ as a parameter. It is seen from this figure that there is no attenuation at all frequencies when the direction of propagation is parallel to the axis of rotation symmetry. Similar behaviour is also observed for $s$-waves when the direction of propagation and/or polarization is parallel to the $z$-axis.

In figure 2(a), we have plotted the normalized shift in phase velocity $(V - V_o)/V_o$ versus the frequency parameter $\chi_{ol}$ for $p$-waves propagating in the $y$-direction. In this case we observe that except at low frequencies, the acoustic wave is virtually nondispersive and that the phase velocity is only approximated by the appropriate continuum theory [8]. As expected, there is a good agreement between the present calculations and the results of Hirsekorn except in the transition region between the Raleigh and the stochastic regions.

Figure 2(b) displays the variation of the shift in phase velocity with inclination of the propagation direction with respect to the $z$-axis at various normalized frequencies. Predictions based on the continuum theory using the Voigt averaged elastic constants and the Hill averaged elastic constants, represented by symbols, are also shown in the same figure. Overall, we notice a good agreement between these predictions and the present results. It is of interest to note that for propagation directions nearly parallel to the axis of rotation symmetry, continuum theory based on the Voigt averaged elastic constants yield results closer to the present calculations than that based on the Hill averaged values. The opposite is true for cases when propagation direction is nearly at right angle to the $z$-axis.

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Fig. 2. Normalized attenuation coefficient for p-waves in model material.
(a) Frequency Dependence: —— present, ○ Hirsekorn; (b) Directional Dependence: \( \chi_{ol} = \)
— 0.1, —— 1, —— 2.5, —— 5, —— 10.

Fig. 3. Normalized attenuation coefficient for p-waves in model material.
(a) Frequency Dependence: —— present, ○ Hirsekorn; (b) Directional Dependence: \( \chi_{ol} = \)
— 0.1, —— 1, —— 2.5, —— 5, —— 10
○ continuum (Hill), ○ continuum (Voigt).
CONCLUSIONS

We have extended the unified theory of Stanke and Kino [2] to determine the propagation constants in a textured polycrystalline material where the crystallites have cubic symmetry. The particular texture considered here assumes that one of the cube axes of each crystallite is aligned in a preferred direction with the other two being randomly oriented, leading to a transversely isotropic medium. Since our formulation is based on the second-order Keller approximation [4], it accounts for some degree of multiple scattering and is valid for all frequencies. Our numerical results agree well, both qualitatively and quantitatively, with other existing theories. To simplify the problem at hand, we have assumed that the grains are equiaxed. We are currently in the process of developing a formulation for the case of the elongated grains.

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