INFLUENCE OF TEXTURE AND GRAIN MORPHOLOGY ON THE TWO-POINT CORRELATION OF ELASTIC CONSTANTS: THEORY AND IMPLICATIONS ON ULTRASONIC ATTENUATION AND BACKSCATTERING

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INTRODUCTION

The discontinuity in the elastic properties at the grain boundaries of a polycrystal controls the attenuation [1] and noise backscattered [2] by an elastic wave propagating through the material. In stochastic theories, which describe the propagation of the mean field in an ensemble of macroscopically identical microstructures, the effects of these discontinuities are quantified by the two-point correlation of elastic constants. It is well known that this correlation, and hence the attenuation and backscttering, is influenced by grain size [3-5] and shape [6], and recent experimental results of Hirao et al [7] imply a strong dependence on preferred grain orientation (texture). The purpose of this paper is to develop the theory necessary to describe these relationships.

We briefly review the stochastic theories of attenuation and backscttering, indicating the central role played by the two-point correlation function. Then we present the theory relating the two-point correlation to the microstructure, with emphasis on the role of the texture. Implications of these results in terms of both understanding attenuation and microstructure and developing new materials characterization techniques are discussed.

RELATIONSHIP OF TWO-POINT CORRELATION TO ULTRASONIC ATTENUATION AND BACKSCATTERING

Stanke and Kino [1] have studied the propagation of an ultrasonic wave in a polycrystal. Utilizing the Keller [8] approximation, they have concluded that the mean field is governed by a stochastic wave equation, which has been cast in the form of a modified Christoffel equation by Ahmed and Thompson [6].

$$
\left|\Gamma_{ik} - \rho \frac{\omega^2}{k^2} \delta_{ik}\right| \hat{u}_k = 0
$$
\n(1)
\nwhere $\Gamma_{ik} = \left\langle \langle C_{ijkl} \rangle + \left[\langle \delta C_{ij\alpha\beta} \delta C_{\gamma\delta kl} \rangle - \langle \delta C_{ij\alpha\beta} \rangle \langle \delta C_{\gamma\delta kl} \rangle \right] \int_{-\infty}^{\infty} G_{\alpha\gamma}(\bar{s}) \left[W(\bar{s}) e^{ik\bar{s}.\bar{k}} \right]_{\beta\delta} dv \right\rangle \hat{k}_i \cdot \hat{k}_1$ (2)

Here the symbol <...> denotes an ensemble average, G is a Green's function, $W(\vec{s})$ is the probability that two points separated by a distance \vec{s} are in the same grain, \hat{u} is the wave polarization, \hat{k} is a unit vector in the direction of propagation, C_{ijkl} is the elastic stiffness tensor and δC_{ijkl} is its deviation from the Voigt average. Solution of this equation for the complex propagation constant k leads to predictions of the velocity v= ω /Re(k) and attenuation α =lm(k).

Rose has studied the noise backscattered as an ultrasonic wave propagating through a polycrystal [3-5].After trivial manipulation [9] his results can be put in the form:

$$
\eta = \frac{\pi^{2}f^{4}}{v_{1}^{2}(\rho v_{1}^{2})^{2}} \Big\langle \delta C_{ijk\delta} C_{pqrs} \Big\rangle \int_{-\infty}^{\infty} W(\vec{s}) e^{2ik\vec{s}\cdot\vec{k}} dv \ \hat{u}_{i}\hat{u}_{k}\hat{u}_{p}\hat{u}_{i}\hat{k}_{j}\hat{k}_{i}\hat{k}_{q}\hat{k}_{s}
$$
\n(3)

where η is the backscattering coefficient. In both equations (2) and (3), the microstructural information is contained in the two-point correlation function, $\langle \delta C_{ijkl} \delta C_{pqrs} \rangle W(\vec{r} - \vec{r})$. In the next section, we will consider in detail the dependence of this function on grain morphology and texture.

INFLUENCE OF TEXTURE AND GRAIN MORPHOLOGY ON THE TWO-POINT CORRELATION OF ELASTIC CONSTANTS

The grain morphology controls the two-point correlation through the factor $W(\vec{r} - \vec{r})$. This will depend on the distribution of grain size and shape as shown in Fig. 1 (a). For equi-axed grains (Fig. 1b.), an approximation that has been commonly used because of its analytical simplicity and reasonable description of typical microstructures is the function

$$
W(\vec{r} - \vec{r}) = e^{-2|\vec{r} - \vec{r}|}/d
$$
\n(4)

Ahmed and Thompson [6] have proposed a generalization to the $W(\vec{r} - \vec{r})$ form for elongated grains (Fig. 1c.):

$$
W(\vec{r} - \vec{r}) = e^{-2|\vec{r} - \vec{r}|} \left(\frac{1}{d^2} \sin^2 \theta + \frac{1}{h^2} \cos^2 \theta \right)^{1/2}
$$
 (5)

Preferred grain orientation enters the theory through the factor $\langle \delta C_{\text{ijkl}} \delta C_{\text{pqs}} \rangle$. The major

contribution of this paper is the evaluation of the influence of preferred grain orientation (texture) on this quantity. By way of background, it is necessary to review a few concepts in quantitative texture analysis. The orientation of a crystallite in a microstructure may be specified by means of Euler angles θ , ψ , and ϕ as shown in Fig. 2a. The orientation distribution function (ODF), the probability density that a crystallite's orientation is given by a prescribed set of Euler angles, is then represented by $w(\xi, w, \phi)$ [10], where $\xi = \cos\theta$ and

Fig. 1. (a) Typical grain size and shape distribution (b) Equiaxed grains with chord length having Poisson's statistics. (c) Elongated grains.

$$
\int_0^{2\pi} \int_0^{2\pi} \int_{-1}^1 w(\xi, \psi, \varphi) d\xi d\psi d\varphi = 1
$$

The orientation distribution function may be written in terms of the orientation distribution

coefficients (ODC's),
$$
W_{lmn}
$$
, and the generalized spherical harmonics as follows:
\n
$$
w(\xi, \psi, \varphi) = \sum_{i=0}^{\infty} \sum_{m=-1}^{i} \sum_{n=-1}^{i} W_{lmn} Z_{lmn}(\xi) e^{-im\psi} e^{-in\phi}
$$
\n(7)

where Z_{Imn}(5) is the generalization of the associated Legendre function [10-11]. In practice, due to sample and crystalline symmetry, only a few of the ODC's are nonzero. In the stochastic model, the elastic stiffnesses correlation function is given by the following expression:

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\n
$$
\langle \delta C_{ijkl} \delta C_{pqrs} \rangle = \int_0^{2\pi} \int_0^2 \int_{-1}^1 \left[\delta C_{ijkl}(\xi, \psi, \varphi) \delta C_{pqrs}(\xi, \psi, \varphi) \right] w(\xi, \psi, \varphi) d\xi d\psi d\varphi
$$

(8)

where $\delta C(\xi,\psi,\phi)$ is obtained by a tensor rotation of the crystalline axes with respect to the sample axes defined by the Euler angles. Because $\langle \delta C_{ijkl} \delta C_{pqrs} \rangle$ transforms as an eight rank tensor, only ODC's of order I<8 will remain when Eq. (8) is evaluated. Recall that $\delta C_{ijkl} = C_{ijkl} - C_{ijkl}$ where C_{ijkl} is a component of the elastic constant tensor of a single grain and $\langle C_{ijkl} \rangle$ is the corresponding component of the ensemble average of the elastic constant tensor of a polycrystal. Expressions for δC_{ijkl} based on the Voigt averaging method have been developed for both hexagonal and cubic crystallites [12-13]. Results for $\left\langle \delta C_{ijkl} \delta C_{pqrs} \right\rangle$ have been developed by Hirsekorn for cubic crystallites [14].

In this paper, we will give explicit forms for the elastic constant correlations pertinent to backscattering for longitudinal or transverse waves propagating along the 1, 2 or 3 directions of aggregates of hexagonal crystallites. Examination of Eq. (3) shows that these are the tensor components <8C_{mnmn} 8C_{mnmn}> where the wave is propagating in the n-direction and is polarized in the m-direction and a summation over identical indices is not implied by the notation.

Fig. 2. (a) The orientation of a crystallite in a polycrystalline sample having axes RD, TO, and NO specified by the means of the Euler angles. (b) The rotation of the sample reference system.

(6)

Consider first the case of longitudinal waves propagating in the 3-direction. The relevant tensor component, C₃₃₃₃ in the specimen coordinate system, may be expressed in terms of the single crystal elastic constants of that grain with respect to its own principal axes, C_{IJ,} and the Euler angles using the rotational transformation and the elastic stiffness matrices given in [15]. Here we have used the matrix notation for the single crystal elastic constants, to differentiate them from the tensor components of rotated crystallites and ensemble averages. For example, C₃₃₃₃ and <C₃₃₃₃> for a hexagonal material are given by:

$$
C_{3333} = C_{11} + 2\left(-C_{11} + C_{13} + 2C_{44}\right)\cos^{2}(\theta) + \left(C_{11} - 2C_{13} + C_{33} - 4C_{44}\right)\cos^{4}(\theta)
$$
\n(10)

$$
\langle C_{3333} \rangle = \left(8C_{11} + 4C_{13} + 3C_{33} + 8C_{44} \right) / 15
$$
 (11)

Combination of Eqs. (7-11), taking advantage of the orthonormality properties of the generalized spherical harmonics, and performing the integration using MATHEMATICA leads to the following results.

$$
\left\langle \delta C_{3333}^{2} \right\rangle = L3H_{00}W_{000} + L3H_{20}W_{200} + L3H_{40}W_{400} + L3H_{60}W_{600} + L3H_{80}W_{800} \qquad (12)
$$
\nwhere,
\n
$$
L3H_{00} = 4\pi^{2}Z_{00} \begin{bmatrix} 32\left(12C_{11}^{2} - 8C_{11}C_{13} + 3C_{13}^{2} - 16C_{11}C_{33} + 2C_{13}C_{33} + 1/2C_{44}^{2} \right) \end{bmatrix} \qquad (12)
$$
\n
$$
L3H_{20} = 4\pi^{2}Z_{20} \begin{bmatrix} 128\left(8C_{11}^{2} + 12C_{11}C_{13} - C_{13}^{2} - 28C_{11}C_{33} - 10C_{13}C_{33} + 1/2C_{44}^{2} \right) \end{bmatrix}
$$
\n
$$
L3H_{40} = 4\pi^{2}Z_{40} \begin{bmatrix} 128\left(8C_{11}^{2} + 12C_{11}C_{13} - C_{13}^{2} - 28C_{11}C_{33} - 10C_{13}C_{33} + 1/2C_{14}^{2} \right) \end{bmatrix}
$$
\n
$$
L3H_{40} = 4\pi^{2}Z_{40} \begin{bmatrix} 512\left(508C_{11}^{2} + 48C_{11}C_{13} + 17C_{13}^{2} - 1064C_{11}C_{33} - 82C_{13}C_{33} + 1/2C_{14}^{2} \right) \end{bmatrix}
$$
\n
$$
L3H_{60} = 4\pi^{2}Z_{60} \begin{bmatrix} 2048\left(-8C_{11}^{2} + 17C_{11}C_{13} - 2C_{13}^{2} - C_{11}C_{33} - 13C_{13}C_{33} + 1/6C_{44}^{2} \right) \end{bmatrix}
$$
\n
$$
L3H_{60} = 4
$$

where $z_{00} = \sqrt{2}/a$, $z_{20} = \sqrt{10}/a$, $z_{40} = \sqrt{2}/6$, $z_{60} = \sqrt{26}/a$, $z_{80} = \sqrt{34}/a$ and where $W_{000} = \sqrt{2}/8\pi^2$ is a constant.

To determine the elastic constant correlations pertinent to longitudinal waves propagating in the 1 & 2-directions, the elastic constants correlation function may be evaluated by rotating the sample coordinate system by α , β , and γ as shown in Fig. 2b. The new ODC's, W'_{lmn}, may then be evaluated from the old ODC's, W_{lmn} according to: [11]

$$
W_{1mn} = \left(\frac{2}{2l+1}\right)^{1/2} \sum_{p=-l}^{l} W_{1mn} Z_{1mn} \left(\cos \beta\right) e^{-ip\alpha} e^{-im\gamma}
$$
 (13)

Thus. we are able to find expressions for the elastic constants correlation functions for the three principle propagation directions in the sample. The results are:

$$
W'_{000} = W_{000} \tag{14}
$$

$$
W'_{200} = \left(\frac{2}{5}\right)^{1/2} \left(-z_{20}W_{200} - z_{22}W_{220}\right)
$$
 (15)

$$
W'_{400} = \left(\frac{2}{7}\right)^{1/2} \left(3 \, z_{40} W_{400} \, \frac{1}{2} \, 2z_{42} W_{420} + 2z_{44} W_{440}\right) \tag{16}
$$

$$
W'_{600} = \left(\frac{2}{9}\right)^{1/2} \left(-5 \, z_{60} W_{600} - \frac{2z_{62} W_{620} + 2z_{64} W_{640} - 2z_{66} W_{660}}{17}\right) \tag{17}
$$

$$
W'_{800} = \left(\frac{2}{11}\right)^{1/2} \left(35 \, z_{80} W_{800} + 2 z_{82} W_{820} + 2 z_{84} W_{840} + 2 z_{86} W_{860} + 2 z_{88} W_{880}\right) \tag{18}
$$

where z_{20} , z_{40} , z_{60} , and z_{80} are the same as before and where $z_{22} = \sqrt{15}/14$, $z_{42} = \sqrt{5}/8$, $z_{44} = \sqrt{35}/16$, $Z_{62} = \sqrt{2730}/_{64}$, $Z_{64} = \sqrt{91}/_{32}$, $Z_{66} = \sqrt{6006}/_{64}$, $Z_{82} = \sqrt{1196}/_{128}$, $Z_{84} = \sqrt{1309}/_{128}$, $Z_{86} = \sqrt{14586}/_{128}$, $Z_{88} = \sqrt{12155}/_{256}$. Note that the top sign of the (\pm) symbol which is used in these equations is for the 1-direction and the bottom sign refers to the 2-direction. Thus $<8C^2_{1111}$ and $<8C^2_{2222}$ are obtained by replacing W_{imn} by W'_{lmn} in the right-hand side of equation (12), where the W'_{lmn} are given by Eqs. (14)-(18) with the upper sign pertaining to the 1-direction and the lower sign to the 2-direction.

Next the elastic constant correlation functions for a transverse wave propagating in the 3 direction and polarized in the 1 and 2 directions in an aggregate of hexagonal crystallites are:

$$
\left\langle \delta C_{13i3}^{2} \right\rangle = T2H_{00}W_{000} + T2H_{20}W_{200} + T2H_{22}W_{220} + T2H_{40}W_{400} + T2H_{42}W_{420} + T2H_{44}W_{440} + T2H_{60}W_{600} + T2H_{64}W_{640} + T2H_{80}W_{800} + T2H_{82}W_{820} + T2H_{84}W_{840}
$$
\n
$$
(19)
$$

where the upper of the $\frac{1}{2}$ sign is used when i=1 and the lower sign is used when i=2 and where,

$$
T2H_{00} = 4\pi^2 z_{00} \begin{pmatrix} 23C_{11}^2 - 50C_{11}C_{12} + 35C_{12}^2 + 8C_{11}C_{13} - 40C_{12}C_{13} + 32C_{13}^2 - 4C_{11}C_{33} + 20C_{12}C_{33} \\ -32C_{13}C_{33} + 8C_{33}^2 - 84C_{11}C_{44} + 60C_{12}C_{44} + 48C_{13}C_{44} - 24C_{33}C_{44} + 108C_{44}^2 \end{pmatrix} / 1575
$$

r.

$$
T2H_{20} = 4\pi^2 z_{20}\n\begin{pmatrix}\n-25C_{11}^2 + 88C_{11}C_{12} - 55C_{12}^2 - 76C_{11}C_{13} + 44C_{12}C_{13} + 32C_{13}^2 + 38C_{11}C_{33} - 22C_{12}C_{33} \\
-32C_{13}C_{33} + 8C_{33}^2 + 24C_{11}C_{44} - 132C_{12}C_{44} + 216C_{13}C_{44} - 108C_{33}C_{44} + 84C_{44}^2\n\end{pmatrix}\n\begin{pmatrix}\n-25C_{11}^2 + 25C_{12}^2 + 24C_{11}C_{13} + 44C_{12}C_{13} + 24C_{13}C_{14} - 108C_{13}C_{14} - 108C_{1
$$

$$
T2H_{22} = 4n^{2}z_{22} = 4n^{2}z_{23} = 4n^{2}z_{24} = 4n^{2}z_{4} =
$$

Finally, the elastic constants correlation function for a transverse wave propagating in the 1-direction and polarized in the 2- direction is:

$$
\left\langle \delta C_{1212}^2 \right\rangle = T1H_{00}W_{000} + T1H_{20}W_{200} + T1H_{40}W_{400} + T1H_{44}W_{440} + T1H_{60}W_{600} + T1H_{64}W_{640} + T1H_{80}W_{800} + T1H_{84}W_{840} + T1H_{88}W_{880}
$$
\n
$$
(20)
$$

where, $TH_{00} = T2H_{00}$

$$
THH_{20} = 4\pi^{2}Z_{20}
$$
\n
$$
33\left(25C_{11}^{2} - 88C_{11}C_{12} + 55C_{12}^{2} + 78C_{11}C_{13} - 44C_{12}C_{13} - 32C_{13}^{2} - 38C_{11}C_{33} + 22C_{12}C_{33} - 42C_{13}C_{33} - 24C_{11}C_{44} + 132C_{12}C_{44} - 216C_{13}C_{44} + 108C_{33}C_{44} - 84C_{44}^{2} - 172C_{43} + 104C_{44} + 104C_{44}^{2} - 516C_{11}C_{33} + 104C_{12}C_{33} - 1048C_{13}C_{33} + 282C_{33}^{2} - 148C_{44}^{2} + 104C_{43}^{2} - 516C_{11}C_{33} + 104C_{12}C_{33} - 1048C_{13}C_{33} + 282C_{33}^{2} - 148C_{44}^{2} - 4438C_{11}C_{44} + 442C_{12}C_{12}C_{44} + 32C_{13}C_{44} - 16C_{33}C_{44} + 4452C_{44}^{2} - 1672C_{33} + 44C_{44} - 1672C_{44} + 4452C_{44}^{2} - 1672C_{44} + 4452C_{44}^{2
$$

CONCLUSION

Analytical expressions have been presented for the two-point correlation of elastic constants, quantities which control ultrasonic attenuation and backscattering, for the case of a single-phase, aggregates of hexagonal crystallites in which the orientation of crystallines are independent of one another, but not necessarily random. The result show that the correlation is described by two factors which respectively describe the effects of grain size and shape, Eq. (4-5), and preferred orientation, Eqs. (8, 12, 19-20). Either of these can be anisotropic and hence describe of directional dependence of the attenuation/noise.

Particular emphasis has been placed here on the effects of preferred orientation, Since the analytical results are somewhat intimidating, we have evaluated the weights of the ODC's in an expansion of $\langle \delta C_{ijkl} \delta C_{pqrs} \rangle$ for various propagation and polarization directions in titanium as shown in Table I. It can be seen that the weights gradually decrease as the order of the ODC's increases, but the rate of decrease is quite different for different wave types. The seventh column shows the W_{imn} observed in a particular rolled sheet of titanium [16]. The final column shows the product of these W_{imn} and the coefficients for the particular case of a longitudinal wave propagating in the 3direction. Included in the calculation were all W_{Imn} for $1 \le 8$, although only a subset of these were listed in Ref. [16]. Because the W's themselves decrease as well as their weights, the contributions of the higher order terms is less than would be implied by the weights alone.

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