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Yan Li
Iowa State University

R. Bruce Thompson
Iowa State University

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Abstract

Ultrasonic techniques have recently been applied to the texture characterization in polycrystalline aggregates of hexagonal crystals. The basis of this application lies in the relations between the elastic constants $_{ij}$ of the aggregates, which can be inferred from ultrasonic wave velocity measurements, and the orientation distribution coefficients. This communication presents such relations for aggregates which possess orthotropic material symmetry and hexagonal crystal symmetry for Voigt, Reuss, and Hill averaging methods in a unified and concise representation.

Keywords

elastic constants, hexagonal lattices, polycrystals, agglomeration, texture, ultrasonic waves, elasticity

Disciplines

Engineering Mechanics | Engineering Science and Materials | Materials Science and Engineering | Structures and Materials

Comments

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Relations between elastic constants C_{ij} and texture parameters for hexagonal materials

Yan Li and R. Bruce Thompson
Ames Laboratory, Iowa State University, Ames, Iowa 50011

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Ultrasonic techniques have recently been applied to the texture characterization in polycrystalline aggregates of hexagonal crystals. The basis of this application lies in the relations between the elastic constants $\overline{C}_{ij}$ of the aggregates, which can be inferred from ultrasonic wave velocity measurements, and the orientation distribution coefficients. This communication presents such relations for aggregates which possess orthotropic material symmetry and hexagonal crystal symmetry for Voigt, Reuss, and Hill averaging methods in a unified and concise representation.

There has been increasing interest in characterization of texture in hexagonal materials in recent years.[1,2] Texture, or preferred orientation of grains, is often quantitatively described by the orientation distribution coefficients (ODCs) or W_{lmn} in Roe's notation.[3,4] These are, in essence, the coefficients of an expansion of the crystallite orientation distribution function in terms of a series of generalized spherical harmonics. Now, ultrasonic techniques are being applied to texture measurement of hexagonal materials because of their nondestructive nature.[5,6] The foundation of application of ultrasonic techniques to the determination of texture in polycrystalline aggregates of hexagonal crystals lies in the relations between the elastic constants $\overline{C}_{ij}$ of the aggregates, which can be inferred from velocity measurements, and the ODCs. This note presents such relations for aggregates which possess orthotropic material symmetry and hexagonal crystal symmetry.

In general, the elastic constants $\overline{C}_{ij}$ and the elastic compliances $\overline{S}_{ij}$ of a textured material can be formally expressed as

$$\overline{C}_{ij} = C^0_{ij} + \Delta C_{ij}, \tag{1}$$

$$\overline{S}_{ij} = S^0_{ij} + \Delta S_{ij}, \tag{2}$$

where C^0_{ij} and S^0_{ij} are elastic constants and compliances of the corresponding isotropic (texture-free) polycrystalline aggregates satisfying the $C^0_{11} - C^0_{12} = 2C^0_{44}$ and $S^0_{11} - S^0_{12} = \frac{1}{2}S^0_{44}$ isotropy conditions. ΔC_{ij} and ΔS_{ij} are the differences due to the presence of texture; they are functions of W_{lmn} for $0 < l \leqslant 4$. For aggregates of hexagonal crystallites, W_{200}, W_{220}, W_{400}, W_{420}, and W_{440} are the only five independent members of these ODCs which are nonzero.

The explicit relations described by Eqs. (1) and (2) depend on the averaging procedures. Voigt, Reuss, and Hill averaging methods are the three commonly employed in texture study owing to their simplicity. The relations between the elastic constants $\overline{C}_{ij}$ and W_{lmn} for the Voigt averaging method were developed by Sayers.[7] These relations, although explicit in principle, rely on the equations given in the appendix of the paper by Smith and Dahlen.[8] We also independently developed the $\overline{C}_{ij}$-W_{lmn} relations using the method described by Morris.[9] A comparison with the results by Sayers reveals that Sayers' expressions can be further simplified to ours if a print error in the expression for γ_{1111} in the appendix of Smith and Dahlen's paper is corrected. The correct expression for γ_{1111} is

$$\gamma_{1111} = 3\gamma_s^{00c} + 6\gamma_s^{20c} + 6\gamma_s^{22c} + 3\gamma_s^{40c} + \gamma_s^{42c} + \gamma_s^{44c}.$$

To many users of these relations, this error might not be obvious, and further errors might be introduced as a consequence of applying these relations. One of the primary purposes of this communication is to correct that error by explicitly presenting the resulting relations in a form believed to be particularly convenient.

The relations between elastic compliances $\overline{S}_{ij}$ and W_{lmn} for the Reuss averaging method were also derived and published by Sayers,[10] following the procedures outlined by Morris.[9] Practically speaking, ultrasonic velocities are more easily expressed in terms of elastic stiffnesses rather than elastic compliances; and the Hill averaging method, which is the arithmatic mean of the Voigt and Reuss averaging method, is found to give most acceptable accuracy among the three. Hill[11] did not explicitly propose such an averaging method for aggregates of hexagonal crystallites. The definition for Hill's averaging method here is a natural extension from that for aggregates of cubic crystallites, which was proposed by Hill. For this reason, it is often more convenient to invert the $\overline{S}_{ij}$-W_{lmn} relations in Eq. (2) for the Reuss averaging method to the $\overline{C}_{ij}$-W_{lmn} relations. This can be mathematically described as

$$\overline{\mathbf{C}} = \overline{\mathbf{S}}^{-1} = (\mathbf{S}^0 + \Delta\mathbf{S})^{-1} = [\mathbf{S}^0(\mathbf{I} + \mathbf{S}^{0\ -1}\Delta\mathbf{S})]^{-1}. \tag{3}$$

In the application of ultrasonics to texture characterization, the anisotropy of the polycrystalline aggregates is sometimes small. Under this weak anisotropy assumption, $\|\mathbf{S}^{0\ -1}\Delta\mathbf{S}\| << 1.0$. Therefore, the inversion process in Eq. (3) can be carried out analytically, arriving at expressions that resemble Eq. (1) in form. Similar work was done for the cubic materials by Hirao *et al.*[12] At the end of this note, a comparison table will be given to show the results of the analytical inversion for a given set of W_{lmn}.

In the following, explicit expressions for both $\overline{\mathbf{C}}_{\text{Voigt}}$ and $\overline{\mathbf{C}}_{\text{Reuss}}$ are summarized in a unified and concise representation where the contributions of W_{2m0} and W_{4m0} can be readily observed:

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$$
\begin{aligned}
\overline{C}_{11} &= C_{11}^0 + 4\pi^2(4A_1\alpha_1 + B\beta_1),\\
\overline{C}_{22} &= C_{11}^0 + 4\pi^2(4A_1\alpha_2 + B\beta_2),\\
\overline{C}_{33} &= C_{11}^0 + 4\pi^2(4A_1\alpha_3 + B\beta_3),\\
\overline{C}_{23} &= C_{12}^0 + 4\pi^2(2A_2\alpha_1 + B\beta_4),\\
\overline{C}_{13} &= C_{12}^0 + 4\pi^2(2A_2\alpha_2 + B\beta_5),\\
\overline{C}_{12} &= C_{12}^0 + 4\pi^2(2A_2\alpha_3 + B\beta_6),\\
\overline{C}_{44} &= C_{44}^0 + 4\pi^2(A_3\alpha_1 + B\beta_4),\\
\overline{C}_{55} &= C_{44}^0 + 4\pi^2(A_3\alpha_2 + B\beta_5),\\
\overline{C}_{66} &= C_{44}^0 + 4\pi^2(A_3\alpha_3 + B\beta_6),
\end{aligned}
\tag{4}
$$

with

$$
\begin{aligned}
\alpha_1 &= \tfrac{1}{210}(\sqrt{10}W_{200} - 2\sqrt{15}W_{220}),\\
\alpha_2 &= \tfrac{1}{210}(\sqrt{10}W_{200} + 2\sqrt{15}W_{220}),\\
\alpha_3 &= -\tfrac{1}{105}\sqrt{10}W_{200},
\end{aligned}
\tag{4a}
$$

and

$$
\begin{aligned}
\beta_1 &= \tfrac{1}{105}(3\sqrt{2}W_{400} - 4\sqrt{5}W_{420} + 2\sqrt{35}W_{440}),\\
\beta_2 &= \tfrac{1}{105}(3\sqrt{2}W_{400} + 4\sqrt{5}W_{420} + 2\sqrt{35}W_{440}),\\
\beta_3 &= \tfrac{8}{105}\sqrt{2}W_{400},\\
\beta_4 &= -\tfrac{4}{105}(\sqrt{2}W_{400} + \sqrt{5}W_{420}),\\
\beta_5 &= -\tfrac{4}{105}(\sqrt{2}W_{400} - \sqrt{5}W_{420}),\\
\beta_6 &= \tfrac{1}{105}(\sqrt{2}W_{400} - 2\sqrt{35}W_{440}),
\end{aligned}
\tag{4b}
$$

where $\overline{C}_{ij}$ and C_{ij}^0 are averaging method dependent; A_1, A_2, A_3, and B, which are elastic anisotropy constants, are also averaging method dependent. For the Voigt averaging method,

$$
\begin{aligned}
C_{11}^0 &= \tfrac{1}{15}(8c_{11} + 3c_{33} + 4c_{13} + 8c_{44}),\\
C_{12}^0 &= \tfrac{1}{15}(c_{11} + 5c_{12} + c_{33} + 8c_{13} - 4c_{44}),\\
C_{44}^0 &= \tfrac{1}{30}(7c_{11} - 5c_{12} + 2c_{33} - 4c_{13} + 12c_{44}),\\
A_1 &= a_1^c = 4c_{11} - 3c_{33} - c_{13} - 2c_{44},\\
A_2 &= a_2^c = c_{11} - 7c_{12} + c_{33} + 5c_{13} - 4c_{44},\\
A_3 &= a_3^c = -5c_{11} + 7c_{12} + 2c_{33} - 4c_{13} + 6c_{44},\\
B &= a_4^c = c_{11} + c_{33} - 2c_{13} - 4c_{44},
\end{aligned}
\tag{4c}
$$

and for the Reuss averaging method,

$$
\begin{aligned}
C_{11}^0 &= (S_{11}^0 + S_{12}^0)/[(S_{11}^0 - S_{12}^0)(S_{11}^0 + 2S_{12}^0)],\\
C_{12}^0 &= -S_{12}^0/[(S_{11}^0 - S_{12}^0)(S_{11}^0 + 2S_{12}^0)],\\
C_{44}^0 &= 1/S_{44}^0,\\
A_1 &= -4C_{44}^{0^2}a_1^s - 14C_{12}^0C_{44}^0a_0^s,\\
A_2 &= -4C_{44}^{0^2}a_2^s + 14C_{12}^0C_{44}^0a_0^s,\\
A_3 &= -4C_{44}^{0^2}a_3^s,\\
B &= -4C_{44}^{0^2}a_4^s,
\end{aligned}
\tag{4d}
$$

where

$$
\begin{aligned}
S_{11}^0 &= \tfrac{1}{15}(8s_{11} + 3s_{33} + 4s_{13} + 2s_{44}),\\
S_{12}^0 &= \tfrac{1}{15}(s_{11} + 5s_{12} + s_{33} + 8s_{13} - s_{44}),\\
S_{44}^0 &= \tfrac{2}{15}(7s_{11} - 5s_{12} + 2s_{33} - 4s_{13} + 3s_{44}),\\
a_0^s &= s_{11} + s_{12} - s_{33} - s_{13},\\
a_1^s &= 4s_{11} - 3s_{33} - s_{13} - \tfrac{1}{2}s_{44},\\
a_2^s &= s_{11} - 7s_{12} + s_{33} + 5s_{13} - s_{44},\\
a_3^s &= -5s_{11} + 7s_{12} + 2s_{33} - 4s_{13} + \tfrac{3}{2}s_{44},\\
a_4^s &= s_{11} + s_{33} - 2s_{13} - s_{44},
\end{aligned}
\tag{4e}
$$

where c_{ij} and s_{ij} are elastic constants and compliances of single hexagonal crystals and are related by

$$
s_{11} = \frac{1}{2}\left(\frac{c_{33}}{c_0} + \frac{1}{c_{11} - c_{12}}\right), \quad s_{12} = \frac{1}{2}\left(\frac{c_{33}}{c_0} - \frac{1}{c_{11} - c_{12}}\right),
$$

$$
s_{33} = \frac{c_{11} + c_{12}}{c_0}, \quad s_{13} = -\frac{c_{13}}{c_0}, \quad s_{44} = \frac{1}{c_{44}},
$$

$$
c_0 = c_{33}(c_{11} + c_{12}) - 2c_{13}^2.
$$

Once the $\overline{\mathbf{C}}_{\text{Voigt}}$ and $\overline{\mathbf{C}}_{\text{Reuss}}$ are determined, $\overline{\mathbf{C}}_{\text{Hill}} = (\overline{\mathbf{C}}_{\text{Voigt}} + \overline{\mathbf{C}}_{\text{Reuss}})/2$ can be readily calculated. Notice that, regardless of averaging methods, the relation $A_1 + A_2 + A_3 = 0$ always exists. In addition, there are the following relations for α_i and β_i:

$$
\begin{aligned}
&\alpha_1 + \alpha_2 + \alpha_3 = 0,\\
&\beta_1 + \beta_2 + \beta_3 + 2(\beta_4 + \beta_5 + \beta_6) = 0,\\
&\beta_1 + \beta_5 + \beta_6 = \beta_2 + \beta_4 + \beta_6 = \beta_3 + \beta_4 + \beta_5 = 0.
\end{aligned}
$$

Table I lists the elastic isotropy and anisotropy con-

TABLE I. Elastic isotropy and anisotropy constants (in GPa).

Material	Method	C_{11}^0	C_{12}^0	C_{44}^0	A_1	A_2	A_3	B
Ti	Voigt	163.93	75.53	44.20	−62.00	−145.00	207.00	23.00
	Hill	162.86	76.07	43.40	−61.80	−141.81	203.61	16.69
	Reuss	161.78	76.60	42.59	−61.60	−138.61	200.21	10.38
Zr	Voigt	145.68	76.16	36.76	−55.80	−6.60	62.40	42.40
	Hill	145.18	72.28	36.45	−49.05	−5.22	54.27	38.99
	Reuss	144.68	72.39	36.14	−42.30	−3.85	46.14	35.59
Zn	Voigt	134.81	41.59	46.61	345.40	100.70	−446.10	−31.60
	Hill	120.68	38.77	40.96	417.33	17.46	−434.79	−76.66
	Reuss	106.55	35.94	35.31	489.25	−65.78	−423.47	−121.73

TABLE II. Elastic constants $\overline{C}_{ij}$ for a given set of W_{lmn} (in GPa). ($W_{200} = 0.014\,328$, $W_{220} = -0.004\,532$, $W_{400} = 0.003\,117$, $W_{420} = -0.003\,411$, and $W_{440} = 0.002\,361$.)

$\overline{C}$	11	22	33	23	13	12	44	55	66
$\overline{C}_V$	160.80	163.55	168.46	71.26	74.56	80.27	47.44	44.18	40.47
$\overline{C}_{R1}$	158.34	161.35	166.12	72.46	75.88	81.23	45.67	42.79	39.09
$\overline{C}_{R2}$	158.71	161.81	166.58	72.20	75.64	81.09	45.91	42.79	39.35
$\overline{C}_{H1}$	159.57	162.45	167.29	71.86	75.22	80.75	46.55	43.48	39.78
$\overline{C}_{H2}$	159.76	162.68	167.52	71.73	75.10	80.68	46.67	43.48	39.91

stants for Voigt, Reuss, and Hill averaging methods for three common hexagonal materials. The single crystal elastic constants of these materials used in the computations are from Ref. 13. Table II lists the elastic constants $\overline{C}_{ij}$ for a given set of W_{lmn} of a Ti plate sample. The rolling history and chemical composition of this Ti sample are unknown since it was purchased directly from a local vender. The W_{lmn} of this sample were obtained from neutron diffraction.[14] In this table, $\overline{C}_V$ and $\overline{C}_{R_1}$ are the elastic constants $\overline{C}_{ij}$ computed from Eqs. (4), $\overline{C}_{R_2}$ are the elastic constants $\overline{C}_{ij}$ obtained by numerically inverting $\overline{S}_{ij}$. $\overline{C}_{H_1}$ and $\overline{C}_{H_2}$ are the mean values of $\overline{C}_V$-$\overline{C}_{R_1}$ and $\overline{C}_V$-$\overline{C}_{R_2}$, respectively. One can see that $\overline{C}_{R_1}$ and $\overline{C}_{R_2}$ are reasonably close; consequently, so are $\overline{C}_{H_1}$ and $\overline{C}_{H_2}$.

One of the distinguished advantages for the representations in Eqs. (4) is the apparent resemblance to the $\overline{C}_{ij}$-W_{lmn} relations for the cubic materials which were published in Ref. 12 and applied widely. In particular, realizing $W_{200} = W_{220} = 0$ for cubic materials, we can obtain the $\overline{C}_{ij}$-W_{lmn} relations for the cubic materials by multiplying β_i in Eqs. (4b) by 3/2. The factor 3/2 is the consequence of lower-order symmetry for cubic crystallites.

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[1]M. J. Philippe, F. Wagner, and C. Esling, in *Proceedings of the Eighth International Conference on Textures of Materials*, edited by J. S. Kallend and G. Gottstein (The Metallurgical Society, Warrendale, PA, 1988), p. 837.
[2]T. M. Holden, R. R. Hosbons, J. H. Root, and E. F. Ibrahim, *Materials Research Society Symposium Proceedings* (Materials Research Society, Pittsburgh, 1989), Vol. 142.
[3]R. -J. Roe, J. Appl. Phys. **36**, 2024 (1965).
[4]R. -J. Roe, J. Appl. Phys. **37**, 2069 (1966).
[5]Y. Li and R. B. Thompson, *Materials Research Society Symposium Proceedings* (Materials Research Society, Pittsburgh, 1989), Vol. 142, p. 83.
[6]Y. Li, R. B. Thompson, and S. S. Lee, in *Review of Progress in Quantitative NDE 9*, edited by O. D. Thompson and D. E. Chimenti (Plenum, New York, 1990) (in press).
[7]C. M. Sayers, Ultrasonics **24**, 289 (1986).
[8]M. L. Smith and F. A. Dahlen, J. Geophys. Res. **78**, 3321 (1973).
[9]P. R. Morris, J. Appl. Phys. **40**, 447 (1969).
[10]C. M. Sayers, J. Nucl. Mater. **144**, 211 (1987).
[11]R. Hill, Proc. Phys. Soc. A **65**, 349 (1952).
[12]M. Hirao, K. Aoki, and H. Fukuoka, J. Acoust. Soc. Am. **81**, 1434 (1987).
[13]R. F. S. Hearmon, in Landolt–Börnstein: *Numerical Data and Functional Relationships in Science and Technology*, Vol. III/1 (Springer, Berlin, 1966), p. 12.
[14]C. M. Sayers (private communication).

High-power, broad-band InGaAsP superluminescent diode emitting at 1.5 μm

Yoshio Noguchi, Hiroshi Yasaka, Osamu Mikami, and Haruo Nagai[a)]
NTT Opto-electronics Laboratories, 3-1 Morinosato Wakamiya, Atsugi-shi, Kanagawa 243-01, Japan

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An InGaAsP superluminescent diode operating at 1.5 μm wavelength is successfully developed using a buried bent absorbing waveguide structure and antireflection coating to suppress lasing mode. Optical characteristics such as high output power (5 mW at 200 mA), broad-band spectral width (60–70 nm), short coherence length (about 30 μm), and low spectral modulation depth (less than 10%) are achieved. Injection current dependence of emitting wavelength and spectral width are also investigated.

Superluminescent diodes (SLDs) have been receiving increasing attention for applications in short and medium distance optical communications. Optical characteristics such as elimination of modal noise in fiber systems, immunity to optical feedback noise, and high coupling efficiency in fibers are of particular interest. SLDs are also a key device in optical fiber gyroscope and optical time domain reflectometry (OTDR) applications.[1,2] The broad-band characteristics of SLDs can reduce Rayleigh backscattering noise and polarization noise in fiber gyro systems, and short coherent length of SLDs can improve spatial resolution in OTDR applications.

In the past few years, several papers have been published on GaAlAs SLDs emitting at 0.8 μm.[3–5] and InGaAsP SLDs at 1.3 μm wavelength.[8–10] However, there have not been any reports on InGaAsP SLDs operating at 1.5 μm wavelength. The 1.5-μm SLDs are often more desirable than 0.8- and 1.3-μm SLDs for obtaining the ultimate sensitivity in these applications because the minimum propagation loss of fibers

a) Present address: Anritsu Corporation, 1800 Onna, Atsugi-shi, Kanagawa 243, Japan.

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