AVERAGING TECHNIQUES AND ULTRASONIC POLE FIGURES

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INTRODUCTION

There is considerable interest in the evaluation of texture via ultrasonic measurements because of the advantages when compared to evaluation by diffraction techniques. First, ultrasonic measurements are much more rapid and have the potential of being used concurrently while processing. Second, ultrasonic measurements are nondestructive while diffraction techniques require coupons to be cut for samples. Third, ultrasonic measurements, like neutron diffraction, sample the bulk of the test material while, in contrast, x-ray diffraction samples a thin surface layer. The primary disadvantage of ultrasonic measurements is that the textural evaluation must be based on a quite limited amount of data whereas diffraction evaluation is normally based upon a very extensive number of measured points. In spite of this disadvantage, research has shown that ultrasonic measurements are potentially useful. Specifically, it has been established [1,2] that during ultrasonic measurements the textural contribution can be distinguished from stress contribution, and it has been shown [3-10] that ultrasonic measurements do give a measure of the type and amount of texture in metal sheet or plate.

The first ultrasonic texture measurement [3] actually sectioned a rolled test piece and measured bulk wave velocities in a variety of directions. Techniques more applicable to nondestructive evaluation have subsequently been investigated; these include [4,5] measurements of acoustic birefringence, Lamb waves, and Rayleigh waves. The optimum technique or combination of techniques remains to be established. The usual approach for texture evaluation has been to describe a crystallite orientation distribution function (CODF) by a mathematical series and to use the ultrasonic measurements to evaluate the expansion coefficients in the series. This CODF can then be projected onto any desired plane to generate a pole figure. The present work is addressed to the averaging procedure which is part of this process.

CODFs and Pole Figures

The following truncated development follows the work of Sayers [11, 12] and Hirao et al [13]. Both Roe [14-16] and Bunge [17] have suggested a series expansion for the mathematical description of CODFs. Thus, with \( w(\xi, \psi, \phi) \) as the CODF for a polycrystalline aggregate, with \( \psi, \theta, \) and \( \phi \)
as the Euler angles between the axes of a crystallite and the sample axes, with \( \xi = \cos \theta \), and with the normalization condition as

\[
\int \int \int w(\xi, \psi, \phi) \ d\xi \ d\psi \ d\phi = 1, \quad (1)
\]

the CODF may be expanded in Roe's notation to yield

\[
w(\xi, \psi, \phi) = \sum_{1=0}^{\infty} \sum_{m=-1}^{m=1} \sum_{n=-1}^{n=1} w_{1mn} Z_{1mn}(\xi) \exp(-im\psi) \exp(-in\phi), \quad (2)
\]

where \( Z_{1mn}(\xi) \) are generalized Legendre functions. The expansion coefficients, \( w_{1mn} \), may be evaluated from the transform

\[
w_{1mn} = \frac{1}{4\pi^2} \int \int \int w(\xi, \psi, \phi) Z_{1mn}(\xi) \exp(i\mu\psi) \exp(in\phi) \ d\xi \ d\psi \ d\phi. \quad (3)
\]

In orthotropic polycrystalline aggregates of cubic crystallites, many of the expansion coefficients are zero or are symmetry-related to others so that, to fourth order, only three coefficients are independent; these are \( w_{400}, w_{420}, \) and \( w_{440} \).

For polycrystalline aggregates, long wavelength ultrasonic velocities measure elastic constants \( \langle c'_{ij} \rangle \) that are averages for the crystallite orientations over the region traversed by the waves. To relate the experimentally measured \( \langle c'_{ij} \rangle \) to the CODF requires an assumption as to the type of averaging that the experimental value represents. Physically, the origin of the problem is the grain boundary constraint between adjacent grains. In general, if adjacent grains are subjected to the same external stress, the resultant distortions in the two grains differ and mismatch when projected onto the grain boundary. Thus the grain boundaries tend to produce gradients in the stress-strain relationships. Mathematically this results from off-diagonal elements in the elastic constant matrix coupling shear and dilational distortions. Extremal values for the averages of the polycrystalline elastic constants can be obtained from Voigt [18] or Reuss [19] averaging. Voigt averaging assumes homogeneous strain and averages over stress. Reuss averaging assumes homogeneous stress and averages over strain. Hill [20] has suggested that an arithmetic mean of these two averages frequently comes very close to experimental values and is, therefore, more realistic.

It will be recognized that for a normalized CODF the average value for any function of the Euler angles is

\[
\langle f \rangle = \int \int \int f(\xi, \psi, \phi) w(\xi, \psi, \phi) \ d\xi \ d\psi \ d\phi. \quad (4)
\]

From this relationship the experimental elastic constants can be expressed in terms of the CODF expansion coefficients. The necessary relationships for cubic crystallites as derived by Hirao et al [13] are as follows:

\[
\begin{align*}
\langle c'_{11} \rangle_i & = (\lambda + 2\mu)_{ii} - 2c_i \delta_i, \\
\langle c'_{22} \rangle_i & = (\lambda + 2\mu)_{ii} - 2c_i \delta_i, \\
\langle c'_{33} \rangle_i & = (\lambda + 2\mu)_{ii} - 2c_i \delta_i, \\
\langle c'_{44} \rangle_i & = \mu_i + c_i \delta_i, \\
\langle c'_{55} \rangle_i & = \mu_i + c_i \delta_i, \\
\langle c'_{66} \rangle_i & = \mu_i + c_i \delta_i, \\
\langle c'_{23} \rangle_i & = \lambda_i + c_i \delta_i, \\
\langle c'_{31} \rangle_i & = \lambda_i + c_i \delta_i, \\
\langle c'_{12} \rangle_i & = \lambda_i + c_i \delta_i.
\end{align*}
\]

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Here the subscript \( i \) refers to the averaging procedure (i.e., Voigt, Hill, or Reuss) and the other terms are defined by

\[
(\lambda+2\mu)_V = c_{11} - 2c/5, \quad \mu_V = c_{44} + c/5,
\]

\[
(\lambda+2\mu)_R = 2(s_{11} + s_{12} - s/5) / [(s_{11} + 2s_{12})(s_{44} + 4s/5)], \quad \mu_R = (s_{44} + 4s/5)^{-1},
\]

\[
(\lambda+2\mu)_H = [(\lambda+2\mu)_V + (\lambda+2\mu)_R]/2, \quad \mu_H = (\mu_V + \mu_R)/2,
\]

\[
c_V = c_{11} - c_{12} - 2c_{44}, \quad c_R = -4\mu_R s, \quad c_H = (c_V + c_R)/2, \quad s = s_{11} - s_{12} - s_{44}/2.
\]

(6)

In these expressions, the unprimed \( c_{11} \)'s are the single-crystal elastic stiffness constants, \( s_{ij} \)'s are the single-crystal compliance constants, \( \lambda \) and \( \mu \) are the Lamé constants, and the subscripts \( V, R, \) and \( H \) refer to Voigt, Reuss, or Hill averages. The CODF contributes only through the \( \delta_i \) values which are averages generated from Eq. 4 and involve direction cosines that interrelate Euler angles and the directions of wave propagation and polarization.

These \( \delta_i \) values are related to the CODF expansion coefficients in the following way:

\[
\delta_1 = -6\sqrt{2} \pi^2 \frac{w_{400}}{35} \left( w_{420} - \frac{2\sqrt{10}}{3} w_{420} + \frac{\sqrt{70}}{3} w_{440} \right),
\]

\[
\delta_2 = -6\sqrt{2} \pi^2 \frac{w_{400}}{35} \left( w_{420} + \frac{2\sqrt{10}}{3} w_{420} + \frac{\sqrt{70}}{3} w_{440} \right),
\]

\[
\delta_3 = -16\sqrt{2} \pi^2 \frac{w_{400}}{35},
\]

\[
\delta_4 = -16\sqrt{2} \pi^2 \frac{w_{400}}{35} + \frac{\sqrt{5}}{2} w_{420},
\]

\[
\delta_5 = -16\sqrt{2} \pi^2 \frac{w_{400}}{35} - \frac{\sqrt{5}}{2} w_{420},
\]

\[
\delta_6 = 4\sqrt{2} \pi^2 \frac{w_{400}}{35} - \sqrt{70} w_{440}.
\]

(7)

It should be emphasized that all variation due to crystallite orientation is in these \( \delta_i \) terms. Since there are six \( \delta_i \)'s and only three expansion coefficients, it is obvious that there must be some redundancy and only three independent measurements must be made. Even so, evaluation of \( W_{400} \) is not done reliably with only Rayleigh or Lamb wave measurements.

RESULTS

To illustrate the lack of reliability in evaluation of \( W_{400} \) with Lamb waves, Table 1 shows some results for Cu and for Al of three different textures. For present purposes, the numbers associated with the Al samples are simply identifiers to distinguish samples of different texture. With the available data there was redundancy in both \( W_{4040} \) and \( W_{4000} \), and evaluations were made of these coefficients with Voigt, Reuss, and Hill techniques. It is obvious that the agreement between equivalent values in the case of \( W_{4040} \) is much better than in the case of \( W_{4000} \). Reliable evaluation of \( W_{4000} \) without resorting to bulk velocity measurements is a problem which remains to be solved. The comparison of ultrasonic pole figures with diffraction pole figures in the next paragraph show that Hill averaging produces better agreement with diffraction data than do either Voigt or Reuss averaging. Hill averages are therefore used in Table 2 where a comparison is made of expansion coefficients from ultrasonic data with expansion coefficients from diffraction data for the same samples as in Table 1.
Table 1. Comparison of Voigt, Reuss, and Hill Average Values for the CODF Expansion Coefficients of Four Different Materials as Evaluated from $S_0$ and $SH_0$ Lamb Waves.

<table>
<thead>
<tr>
<th>Material</th>
<th>$W_{440}(SH_0)V$</th>
<th>$W_{440}(SH_0)R$</th>
<th>$W_{440}(SH_0)H$</th>
<th>$W_{440}(S_0)V$</th>
<th>$W_{440}(S_0)R$</th>
<th>$W_{440}(S_0)H$</th>
<th>$W_{440}(SH_0)V$</th>
<th>$W_{440}(SH_0)R$</th>
<th>$W_{440}(SH_0)H$</th>
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<th>$W_{440}(S_0)R$</th>
<th>$W_{440}(S_0)H$</th>
<th>$W_{440}(S_0)V$</th>
<th>$W_{440}(S_0)R$</th>
<th>$W_{440}(S_0)H$</th>
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</tr>
<tr>
<td>629°F Al</td>
<td>-0.00573</td>
<td>0.00505</td>
<td>0.00303</td>
<td>-0.00303</td>
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<td>675°F Al</td>
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<td>Copper</td>
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</table>

Table 2. Comparison of Hill Averages of CODF Expansion Coefficients from Ultrasonic Data with Expansion Coefficients from X-ray or Neutron Diffraction Data.

<table>
<thead>
<tr>
<th>Material</th>
<th>1100 Al</th>
<th>629°F Al</th>
<th>678°F Al</th>
<th>Copper</th>
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<tr>
<td>$W_{440}(SH_0)H$</td>
<td>-0.00564</td>
<td>0.00497</td>
<td>0.00298</td>
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<tr>
<td>$W_{440}(S_0)H$</td>
<td>-0.00572</td>
<td>0.00543</td>
<td>0.00291</td>
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<tr>
<td>$W_{420}(S_0)H$</td>
<td>-0.00008</td>
<td>-0.00396</td>
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<td>$W_{400}(SH_0)H$</td>
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<td>$W_{400}(S_0)H$</td>
<td>-0.00791</td>
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<td>$W_{400}(SH_0)H$</td>
<td>-0.01175</td>
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<td>$W_{400}(S_0)H$</td>
<td>-0.00986</td>
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<td>-0.00008</td>
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<table>
<thead>
<tr>
<th>Material</th>
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<th>678°F Al</th>
<th>Copper</th>
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<td>x-ray *</td>
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<tr>
<td>$W_{440}$</td>
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<td>0.0069</td>
<td>0.0043</td>
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<td>-0.0033</td>
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<tr>
<td>$W_{400}$</td>
<td>0.00098</td>
<td>0.0097</td>
<td>0.0078</td>
<td>0.00113</td>
</tr>
</tbody>
</table>

<table>
<thead>
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<th>Material</th>
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<th>Copper</th>
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</thead>
<tbody>
<tr>
<td>neutron **</td>
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<tr>
<td>$W_{440}$</td>
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<tr>
<td>$W_{420}$</td>
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<td>$W_{400}$</td>
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* X-ray diffraction evaluation from G. C. Johnson, Univ. of Calif., at Berkeley.
** Neutron diffraction evaluation from G. V. Blessing and R. C. Reno, National Bureau of Standards, Gaithersburg, MD.
Ultrasonic measurements and x-ray pole figure determinations, with Voigt averaging only, had earlier been made on a series of Cu samples that were cold rolled by varying degrees from 50% reduction to 89% reduction and then annealed. Cu was chosen because its anisotropy ratio [21] of \( \frac{2c_{44}}{c_{11} - c_{12}} = 3.6 \) is considerably greater than that of Al at 1.2. This factor of three difference causes the elastic constants of polycrystalline Cu to be considerably more sensitive to averaging procedure and sensitivity to averaging technique was therefore expected to occur also in the pole figures. This expectation was confirmed as can be seen in Figs. 1-3. These figures show comparisons of x-ray pole figures with ultrasonic pole figures from Voigt, Reuss, and Hill averaging. Figure 1 is for Cu after 50% rolling reduction, Fig. 2 after 89% rolling reduction, and Fig. 3 after subsequent annealing. Only one quadrant of each ultrasonic pole figure is shown because the other three quadrants are reproducible by mirror symmetries across the rolling and transverse directions. It seems obvious that there is a significant difference in equivalent ultrasonic pole figures from the three different averaging techniques, and visual comparison shows in every case that the Hill average produces the best symmetry agreement with the corresponding x-ray pole figure.

Fig. 1. Comparison of x-ray and ultrasonic pole figures for rolled Cu with 50% reduction.
Fig. 2. Comparison of x-ray and ultrasonic pole figures for rolled Cu with 89% reduction.
Fig. 3. Comparison of x-ray and ultrasonic pole figures for rolled Cu after subsequent anneal.
ACKNOWLEDGMENT

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REFERENCES

2. R. B. Thompson, S. S. Lee, and J. F. Smith, Ultrasonics, in press.