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Ultrasonic velocities in textured metals

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A brief review is presented of the calculation of elastic properties in textured metals with a view toward ultrasonic velocity studies. Proceeding from the linearized wave equation for elastic materials, the propagation of elastic waves is analysed from the point of view of plane and curved wavefronts to develop an understanding of the roles of phase and group velocities. This theory is applied to the calculation of the three polarizations of ultrasonic waves in Fe/Si transformer steels of various textures.

1. Introduction

The propagation of ultrasonic waves in metals is strongly affected by grain boundaries, porosity, texture and various structural defects. For this reason ultrasound is often used in the non-destructive testing of the quality and mechanical properties of a material. Texture, in particular, strongly affects the anisotropy of elastic properties and thus is of importance in the development of fully quantitative methods for interpreting ultrasonic measurements. Of relevance for such studies is the texture description developed by Bunge [1] and Roe [2] which makes possible the calculation of the polycrystal elastic constants and thus the ultrasonic velocities in polycrystalline aggregates. The calculations for orthorhombic physical symmetry and cubic crystal symmetry were first performed by Morris [3] but a simpler, however less accurate, method has been proposed by Bunge [4]. We deviate from the Roe texture description used by Sayers [5] for his calculation of ultrasonic velocities along the three perpendicular symmetry axes in austenitic stainless steel and utilize this latter method and the Bunge texture description to perform a more comprehensive treatment of ultrasonic velocity anisotropy. Expressions will be derived for the anisotropy of the phase and group velocities and the theory will be applied to Fe/Si specimens of various textures.

2. Elastic constants in polycrystalline textured metals

It is well known that Hook's law, which in one dimension assumes a linear relationship between the force applied to a material and the resulting strain, can be generalized for crystals to the form

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl} \qquad (1)$$

which expresses the stress tensor components σ_{ij} in terms of the strain tensor components ε_{kl} through the elastic constants c_{ijkl} of the crystal. One can also express the strain components in terms of the stress components through the elastic compliances s_{ijkl}

$$\varepsilon_{ij} = s_{ijkl}\sigma_{kl} \qquad (2)$$

which forms the inverse of c_{ijkl}. Although these results are valid for single crystals, they can be adapted to polycrystalline materials by taking averages over the orientation distribution function (ODF)

$$f(g) = \sum_{l=0}^{\infty} \sum_{\mu=1}^{M(l)} \sum_{\nu=1}^{N(l)} C_l^{\mu\nu} T_l^{\mu\nu}(g) \qquad (3)$$

which describes the volume fraction of crystallites in the sample having an orientation specified by the rotation g. Assuming that the strains in all crystallites are the same, one obtains the Voigt approximation for the elastic constants

$$\overline{\sigma_{ij}} = \overline{c_{ijkl}\varepsilon_{kl}} \qquad (4)$$

and assuming that the stresses in all crystallites are the same, one obtains the Reuss approximation for the elastic compliances

$$\overline{\varepsilon_{ij}} = \overline{s_{ijkl}\sigma_{kl}} \qquad (5)$$

Bunge points out that for crystals having cubic symmetry [6] the single crystal elastic tensors can be expressed as a sum of two parts, an isotropic part and an anisotropic part, so that the ODF averaged tensors take the form

$$c_{ijkl}^{\mathrm{V}} = \overline{c_{ijkl}} = c_{ijkl}^{\mathrm{I}} + c_{\mathrm{a}}\overline{t_{ijkl}} \qquad (6)$$

$$s_{ijkl}^{\mathrm{R}} = \overline{s_{ijkl}} = s_{ijkl}^{\mathrm{I}} + s_{\mathrm{a}}\overline{t_{ijkl}} \qquad (7)$$

where only the anisotropic parts of the single crystal tensors appear in the averages. The constants c_{a} and s_{a} measure the amount to which the single crystal tensors deviate from their isotropic counterparts and the crystallite averaged t_{ijkl} tensor is found to be given by

$$\overline{t_{ijkl}} = \overline{a_{ijkl}^{011}} + \overline{a_{ijkl}^{411}}C_4^{11} + \overline{a_{ijkl}^{412}}C_4^{12} + \overline{a_{ijkl}^{413}}C_4^{13} \qquad (8)$$

involving only the $l = 4$ texture coefficients and additional mathematical constants dependent on the sample symmetry being considered.

Improvements to the restrictive assumptions of Voigt and Reuss concerning the elastic behaviour at grain boundaries can be made by following Hill's prescription of taking the average of the tensors obtained by these methods. One obtains

$$c_{ijkl}^{\mathrm{H}} = \tfrac{1}{2}(c_{ijkl}^{\mathrm{V}} + c_{ijkl}^{\mathrm{R}}) \qquad (9)$$

$$s_{ijkl}^{\mathrm{H}} = \tfrac{1}{2}(s_{ijkl}^{\mathrm{V}} + s_{ijkl}^{\mathrm{R}}) \qquad (10)$$

which yields a closer approximation to the true elastic properties of polycrystalline materials.

3. Wave propagation and plane wave solutions

On the basis of a general description of the deformations of linearly elastic materials, a tensor wave equation involving the material's elastic constants and mass density can be derived (Landau and Lifshitz [7]). Its simplified linearized form, which assumes small material displacements and a constant mass density, takes the form

$$\varrho_0 \frac{\partial^2 \boldsymbol{u}_i}{\partial t^2} = c_{ijkl} \frac{\partial^2 \boldsymbol{u}_l}{\partial x_j \partial x_k} \tag{11}$$

where the vector $\boldsymbol{u}_i(\boldsymbol{x}, t)$ describes the dynamic displacement of the material at the equilibrium position $\boldsymbol{x}$. The calculation of the velocities of ultrasonic waves proceeds from this equation by looking for solutions in the form of travelling plane waves

$$\boldsymbol{u}_i(\boldsymbol{x}, t) = \hat{\boldsymbol{\varepsilon}}_i \exp\left[\mathrm{i}(\boldsymbol{k} \cdot \boldsymbol{x} - \omega t)\right] \tag{12}$$

involving a constant polarization vector $\hat{\boldsymbol{\varepsilon}}$. Inserting this equation into the above wave equation results in the matrix expression

$$(c_{ijkl} k_j k_k - \delta_{il} \varrho_0 \omega^2) \varepsilon_i = 0 \tag{13}$$

whose solution requires solving the Christoffel determinant

$$\det\,(c_{ijkl} k_j k_k - \delta_{il} \varrho_0 \omega^2) = 0 \tag{14}$$

One makes use of the changes of variable $k_i = kn_i$ and $v = \omega/k$ to transcribe this equation to the form

$$\det\,(c_{ijkl} n_j n_k - \delta_{il} \varrho_0 v^2) = 0 \tag{15}$$

involving the *phase velocity* v of the plane wave crests and the direction cosines n_i of the propagation vector $\boldsymbol{k}$.

In general, there exists three real roots to this cubic equation, designated $v^\alpha = v^\alpha(n_i)$ for $\alpha = 1, 2, 3$. Each corresponds to one of three orthogonal polarization eigenvectors $\hat{\boldsymbol{\varepsilon}}^\alpha(n_i)$ obtained by inserting the expression for $v^\alpha(n_i)$ into Equation 13 and solving for $\boldsymbol{\varepsilon}_i$. It is important to note, however, that it is the *group velocity* $c_i = \mathrm{d}\omega/\mathrm{d}k_i$ which is the physically relevant quantity to be considered for velocity measurements.

4. Phase and group velocity

We have mentioned that there is a difference between the phase and group velocities for plane waves in anisotropic materials, and it is appropriate that we examine more closely its significance. From an inspection of Equation 15, one can see by making the change of variable $n_i \rightarrow \lambda n_i$ that the solutions of the phase velocity will necessarily have the property

$$v^\alpha(\lambda n_i) = \lambda v^\alpha(n_i) \tag{16}$$

We exploit Euler's identity for homogeneous functions and differentiate with respect to λ to obtain

$$\frac{\partial v^\alpha(\lambda n_i)}{\partial(\lambda n_j)} n_j = v^\alpha(n_i) \tag{17}$$

which, by then setting $\lambda = 1$, results in the expression

$$\frac{\partial v^\alpha(n_i)}{\partial n_j} n_j = c_j^\alpha(n_i) n_j = v^\alpha(n_i) \tag{18}$$

Thus a plane wave moving in the direction $\hat{\boldsymbol{n}}$ with

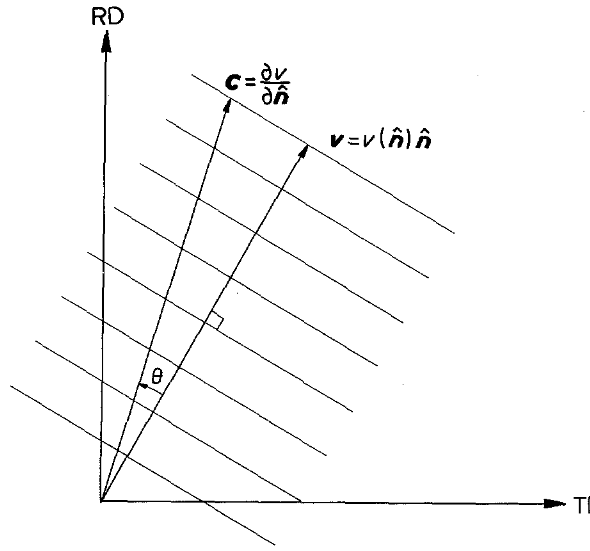

Figure 1 Phase and group velocity vectors for a travelling plane wave.

phase velocity $v^\alpha(\hat{\boldsymbol{n}})$ will have a group velocity vector $\boldsymbol{c}^\alpha(\hat{\boldsymbol{n}})$ such that $\boldsymbol{c}^\alpha(\hat{\boldsymbol{n}}) \cdot \hat{\boldsymbol{n}} = v^\alpha(\hat{\boldsymbol{n}})$. This suggests that unlike the phase velocity, which measures the normal velocity of the wavefront, the group velocity measures the velocity of the wavefront in a direction other than the normal direction – see Fig. 1. The direction itself is determined by the form of $v^\alpha(n_i)$ which depends on the elastic properties of the material being considered.

The physical importance of the group and the phase velocities is not demonstrated in this analysis involving plane wave solutions. Experimentally, one measures the arrival time of an elastic disturbance. As to which quantity is the one relevant for experiments, an analysis based on the more realistic case of curved wavefronts is required. Fundamental to such an analysis is the property that a curved wave surface propagates locally with a velocity equal to that of a plane wavefront moving in the direction of the local surface normal – i.e. $v^\alpha(\hat{\boldsymbol{n}})\,\hat{\boldsymbol{n}}$ [8]. This agrees with our intuition that a curved wave surface can always be considered on a sufficiently small scale as approximating a plane wave. Then, the arrival time of the surface at a particular point $\boldsymbol{x}$ in the material body can be obtained by summing the time increments along the appropriate ray trajectory that describes the time development of the local surface normal

$$t_{\mathrm{ph}} = \int_{C_{\mathrm{ph}}}^{\boldsymbol{x}} \frac{|\mathrm{d}\boldsymbol{x}'|}{|\boldsymbol{v}^\alpha(\boldsymbol{x}')|} \tag{19}$$

Such a curved trajectory will henceforth be called a *phase velocity ray*.

Instead of considering rays that follow the local surface normal of the time developing wavefront – i.e. the phase velocity vector $\boldsymbol{v}^\alpha(\hat{\boldsymbol{n}})$ – one can also consider the trajectories of rays that follow the group velocity vector $\boldsymbol{c}^\alpha(\hat{\boldsymbol{n}})$, so that

$$t_{\mathrm{gr}} = \int_{C_{\mathrm{gr}}}^{\boldsymbol{x}} \frac{|\mathrm{d}\boldsymbol{x}'|}{|\boldsymbol{c}^\alpha(\boldsymbol{x}')|} \tag{20}$$

It is important to note that summing the time increments along such *group velocity rays* must give the same wavefront arrival times as those obtained from phase velocity rays, $t_{\mathrm{gr}} = t_{\mathrm{ph}}$, ensuring the uniqueness

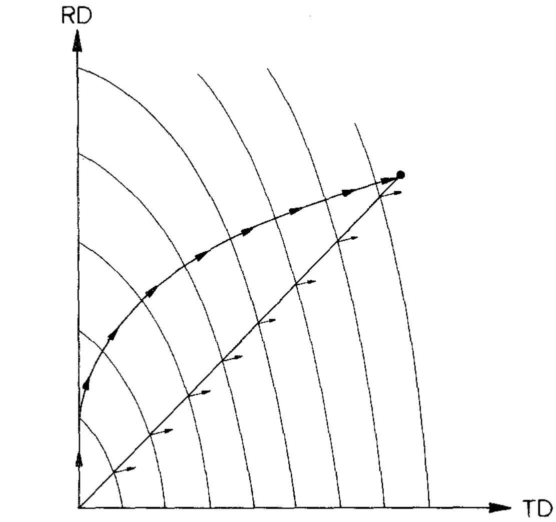

Figure 2 Phase and group velocity rays for a system of curved wavefronts.

of the physical result. As supported by an exhaustive study in the appendix to this paper, group velocity rays are found to be of most importance having the remarkable property that they describe straight line trajectories for even highly distorted wave surfaces (refer to Fig. 2). This happens because the group velocity vector for each surface element is only a function of the surface normal components, $\boldsymbol{c}^\alpha = \boldsymbol{c}^\alpha(\hat{\boldsymbol{n}})$, and these normal vector components remain constant along group velocity rays. Thus, the ray velocity $\boldsymbol{c}^\alpha(\hat{\boldsymbol{n}})$ is a constant along the trajectory C_{gr} and the integral in Equation 20 simplifies to the form

$$t_{gr} = \frac{|\boldsymbol{x}|}{|\boldsymbol{c}^\alpha(\hat{\boldsymbol{n}})|} \tag{21}$$

One then concludes that experimental velocity measurements are really a determination of the group velocity along straight line trajectories.

5. Orthorhombic sample symmetry example

After a demonstration to show that the propagation of ultrasonic waves follows the group velocity of a wave surface we proceed with the explicit calculation of the phase and group velocities for textured specimens of cubic crystal symmetry and orthorhombic sample symmetry. The cumbersome 4-index tensor notation is translated to 2-index matrix notation, Equation 1 becomes

$$\begin{vmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{vmatrix} = \begin{vmatrix} C_{11} & C_{12} & C_{13} & & & \\ C_{12} & C_{22} & C_{23} & & & \\ C_{13} & C_{23} & C_{33} & & & \\ & & & C_{44} & & \\ & & & & C_{55} & \\ & & & & & C_{66} \end{vmatrix} \begin{vmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{vmatrix} \tag{22}$$

By exploiting the symmetry of the tensor of elastic constants

$$c_{ijkl} = c_{ijlk} = c_{jikl} = c_{klij} \tag{23}$$

the assignments can be summarized by

$$C_{11} = c_{1111} \quad C_{12} = c_{1122} \quad C_{44} = c_{2323} \tag{24a}$$

$$C_{22} = c_{2222} \quad C_{13} = c_{1133} \quad C_{55} = c_{1313} \tag{24b}$$

$$C_{33} = c_{3333} \quad C_{23} = c_{2233} \quad C_{66} = c_{1212} \tag{24c}$$

Then, with the following abbreviations

$$A = C_{11}n_1n_1 + C_{22}n_2n_2 + C_{33}n_3n_3 \tag{25a}$$

$$B = C_{11}n_1n_1 + C_{22}n_2n_2 + C_{33}n_3n_3 \tag{25b}$$

$$C = C_{11}n_1n_1 + C_{22}n_2n_2 + C_{33}n_3n_3 \tag{25c}$$

$$D = (C_{12} + 2C_{66})n_1n_2 \tag{25d}$$

$$E = (C_{13} + 2C_{55})n_1n_3 \tag{25e}$$

$$F = (C_{23} + 2C_{44})n_2n_3, \tag{25f}$$

the Christoffel determinant (Equation 15) can be written in the matrix form

$$\det \begin{vmatrix} A - \varrho_0 v^2 & D & E \\ D & B - \varrho_0 v^2 & F \\ E & F & C - \varrho_0 v^2 \end{vmatrix} = 0 \tag{26}$$

In the case of the sample plane where $n_3 = 0$ this determinant simplifies to yield for the phase velocity eigenvalues

$$v^L = \frac{1}{(2\varrho_0)^{1/2}} \{C_{66} + C_{11}n_1^2 + C_{22}n_2^2 + [A^2n_1^4 + B^2n_2^4 + 2n_1^2n_2^2(2C^2 - AB)]^{1/2}\}^{1/2} \tag{27a}$$

$$v^H = \frac{1}{(2\varrho_0)^{1/2}} \{C_{66} + C_{11}n_1^2 + C_{22}n_2^2 - [A^2n_1^4 + B^2n_2^4 + 2n_1^2n_2^2(2C^2 - AB)]^{1/2}\}^{1/2} \tag{27b}$$

$$v^V = \frac{1}{(\varrho_0)^{1/2}} (C_{55}n_1^2 + C_{44}n_2^2)^{1/2} \tag{27c}$$

where we have adopted the abbreviated forms

$$A = C_{11} - C_{66} \quad B = C_{22} - C_{66} \quad C = C_{12} + C_{66} \tag{28}$$

The superscripts L, H and V replacing the Greek letter α have significance arising from the polarization properties in untextured specimens – L corresponding to the polarization along the wavevector $\boldsymbol{k}$, H corresponding to the polarization in the sample plane but perpendicular to the wavevector $\boldsymbol{k}$, and V corresponding to the polarization perpendicular to both the wavevector $\boldsymbol{k}$ and the sample plane.

If the expressions 27 for the phase velocities are differentiated with respect to the n_i, we obtain

$$\boldsymbol{c}^L = \frac{1}{2\varrho_0}\frac{1}{v^L}(g_1^L n_1, g_2^L n_2, 0) \tag{29a}$$

$$\boldsymbol{c}^H = \frac{1}{2\varrho_0}\frac{1}{v^H}(g_1^H n_1, g_2^H n_2, 0) \tag{29b}$$

$$\boldsymbol{c}^V = \frac{1}{\varrho_0}\frac{1}{v^V}(C_{55}n_1, C_{44}n_2, 0) \tag{29c}$$

TABLE I Texture data for the Fe/Si steel specimens used for ultrasonic velocity calculations

$C_l^{\mu\nu}$	A	B	C
C_4^{11}	0.008	0.67	−1.28
C_4^{12}	−6.186	−1.01	−5.74
C_4^{13}	3.61	−1.51	1.59

for the group velocities where again we have introduced some abbreviated forms

$$g_1^{L} = C_{11} + C_{66} + \frac{A^2n_1^2 + (2C^2 - AB)n_2^2}{[A^2n_1^4 + B^2n_2^4 + 2n_1^2n_2^2(2C^2 - AB)]^{1/2}} \quad (30a)$$

$$g_2^{L} = C_{22} + C_{66} + \frac{B^2n_2^2 + (2C^2 - AB)n_1^2}{[A^2n_1^4 + B^2n_2^4 + 2n_1^2n_2^2(2C^2 - AB)]^{1/2}} \quad (30b)$$

$$g_1^{H} = C_{11} + C_{66} - \frac{A^2n_1^2 + (2C^2 - AB)n_2^2}{[A^2n_1^4 + B^2n_2^4 + 2n_1^2n_2^2(2C^2 - AB)]^{1/2}} \quad (30c)$$

$$g_2^{H} = C_{22} + C_{66} - \frac{B^2n_2^2 + (2C^2 - AB)n_1^2}{[A^2n_1^4 + B^2n_2^4 + 2n_1^2n_2^2(2C^2 - AB)]^{1/2}} \quad (30d)$$

In textured specimens the polarization properties outlined above remain only approximate as can be verified by a calculation of the eigenvectors for each of the velocity eigenvalues of Equation 27. For this reason the superscripts L, H and V are understood to imply quasi-longitudinally polarized waves, etc.

6. Texture measurements and velocity analysis

We have applied the results of our studies to the theoretical prediction of the ultrasonic velocities in Fe/Si transformer steels. Specimens of three different textures were chosen, all being secondary recrystallization textures with large grain size. The specimens were previously used by one of the authors in his investigation of texture influence on magnetic property anisotropy. In order to obtain reliable statistics for the number of grains, neutron diffraction was used. This method is discussed in detail in a review on neutron diffraction and texture [9]. The applicability of this method to our specimens is evident since the volume which can be investigated using neutrons is usually 10^5 times greater than that achieved by X-rays. Thus, even grain sizes of several millimeters could be measured. It was necessary to reduce the effect of neutron primary extinctions, which often limit the diffraction volume to the skin surface of grains in perfect crystals like Fe/Si steels, by using light plastic deformations. This reduces crystal perfection and does not disturb the specimen texture. The crystal orientation distribution functions were calculated from 110, 200 and 211 pole figures and the resulting $C_l^{\mu\nu}$ texture coefficients are listed in Table I. The texture of specimen A was very strong, the density of the orientation distribution at maximum being 70X random which corresponds to Goss texture. Specimens B and C were non-oriented and annealed and represent more complex recrystallization textures.

TABLE II Single crystal elastic constants and mass density

$\varrho_0 = 7.860\,\mathrm{g\,cm^{-3}}$
$C_{11} = 2.331 \times 10^{11}\,\mathrm{N\,m^{-2}}$
$C_{12} = 1.354 \times 10^{11}\,\mathrm{N\,m^{-2}}$
$C_{14} = 1.178 \times 10^{11}\,\mathrm{N\,m^{-2}}$

The calculation of the velocities for the three ultrasonic wave polarizations were performed for these texture specimens. The phase velocities were calculated in sample plane directions in 5° intervals from the rolling direction (RD) and the group velocities were determined in magnitude and direction from these results by using Equations 29 and 30. Use was made of the Hill averaged elastic constants for the entire analysis. Included in Table II are the single crystal elastic constants and mass density also used.

Reference to Fig. 3 confirms the expected result that the group and phase velocities are the same for propagation directions corresponding to the symmetry axes of the specimen (RD) and (TD). For other directions the general behaviour is the same except that the group velocities are consistently less than the phase velocities. This is well exemplified in the horizontal shear velocity for texture B (Fig. 3c) where the shape of the curve is significantly altered even though the texture is quite mild. In the case of the vertical shear velocity for the strongly textured sample A (Fig. 3b) the difference is as high as 20% of the degree of anisotropy. Clearly attention must be paid to group velocity considerations for ultrasonic velocity measurements in textured specimens.

For curiosity sake, we point out that for the calculation of v^{H} and c^{H} in the Goss textured specimen A (Fig. 3d) that something quite unusual occurs. The direction of the group velocity vector is not a single-valued function of the phase velocity direction but instead loops back onto itself. More precisely, as the direction of the phase velocity vector approaches the specimen symmetry axes, the direction of the group velocity vector is found to cross the axes direction before assuming the colinear relationship at $\alpha = 0°$, 90°. The occurrence of this behaviour might indicate that the conditions for simple wave propagation cease to be valid for such strongly textured specimens. Perhaps irregular phenomenon such as wavefront instability, mixing of the various pure wave polarizations or even the development of weak shock phenomena are responsible for this phenomenon.

7. Conclusion

We have presented a concise picture of the important concepts related to ultrasonic velocity calculations in textured materials, having stressed the need to consider the group velocity rather than the phase velocity for even mild textures. Since differences can be appreciable for any of the chosen specimens we restate that the use of ultrasound in material testing requires that data interpretation be carried out in light of a correct

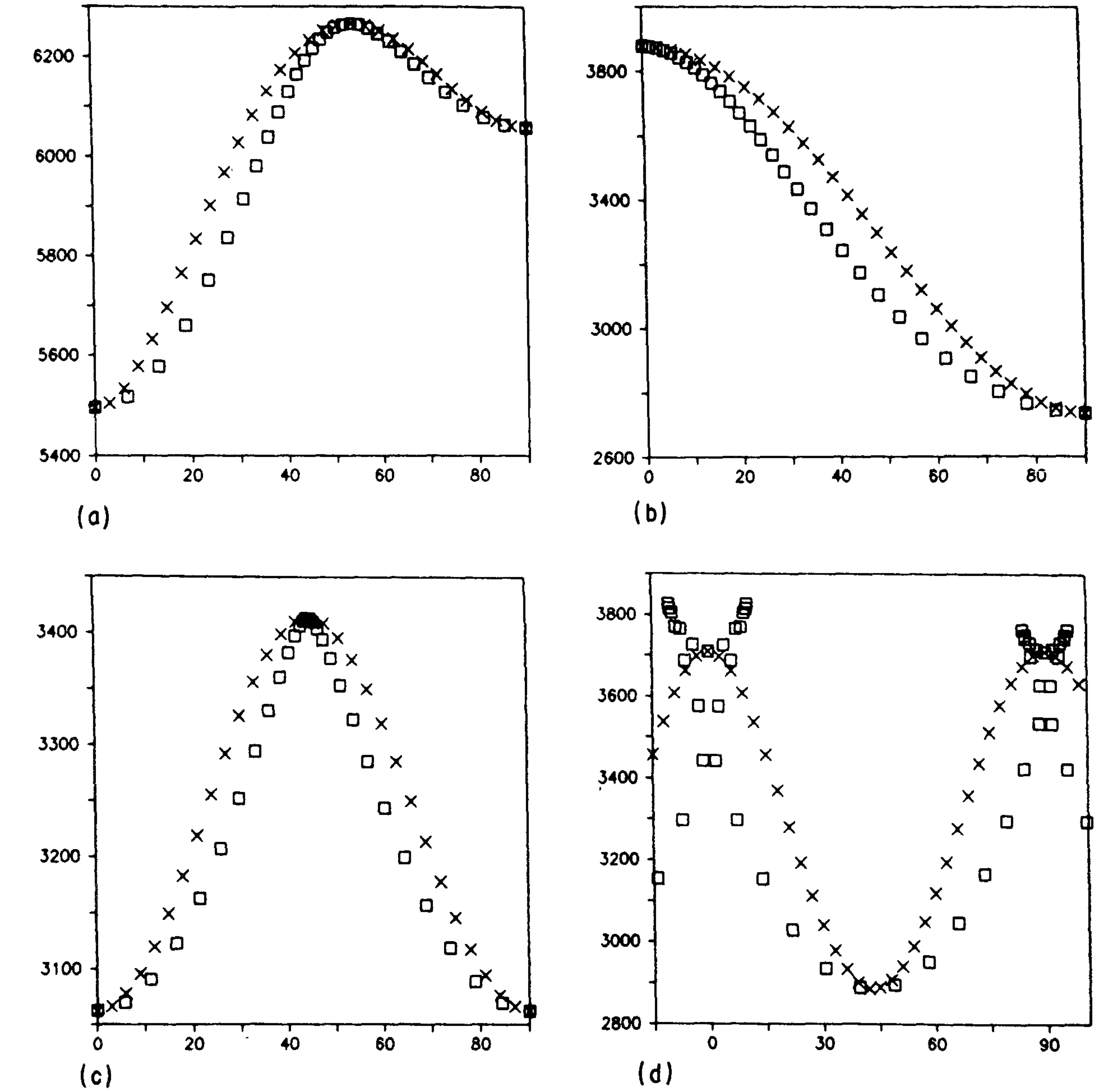

Figure 3 Phase and group velocities as a function of angle from the rolling direction for textured Fe/Si specimens: (a) longitudinal velocities for specimen A, (b) vertical shear velocities for specimen A, (c) horizontal shear velocities for specimen B and (d) horizontal shear velocities for specimen A (□ group, × phase).

understanding of the properties involved in anisotropic wave phenomena.

Appendix A: Kinematics of a moving wavefront

This appendix is concerned with the derivation of an important property of the rays directed along the group velocity of a moving wavefront. To parallel the discussion given by Eringen and Suhubi [10], we introduce at time t a surface $\sigma(t)$ comprised of all points $\boldsymbol{x}$ having a parametrization

$$\boldsymbol{x} = \boldsymbol{x}(\xi^\alpha, t) = x_i(\xi^\alpha, t)\hat{a}_i \tag{A1}$$

involving the curvilinear surface coordinates ξ^α, ($\alpha = 1, 2$) – see Fig. 4. Let the parametrization be such that for any infinitessimal displacement $\mathrm{d}\boldsymbol{x}$ along the surface

$$\mathrm{d}x_i = \frac{\partial x_i}{\partial \xi^\alpha}\mathrm{d}\xi^\alpha \equiv \partial_\alpha x_i \mathrm{d}\xi^\alpha \tag{A2}$$

$$\mathrm{d}\boldsymbol{x} = \hat{\boldsymbol{e}}_\alpha \mathrm{d}\xi^\alpha \tag{A3}$$

where the $\hat{\boldsymbol{e}}_\alpha$ are unit basis vectors on the surface. It is clear that the $\hat{\boldsymbol{e}}_\alpha$ will also have a parametrization $\hat{\boldsymbol{e}}_\alpha = \hat{\boldsymbol{e}}_\alpha(\xi^\beta, t)$. The distance element for this tangential displacement is given by

$$\mathrm{d}s^2 = \mathrm{d}x_i\mathrm{d}x_i = \partial_\alpha x_i \partial_\beta x_i \mathrm{d}\xi^\alpha \mathrm{d}\xi^\beta \tag{A4}$$

$$= g_{\alpha\beta}\mathrm{d}\xi^\alpha \mathrm{d}\xi^\beta \tag{A5}$$

which introduces the surface metric tensor $g_{\alpha\beta}$

$$g_{\alpha\beta} = \partial_\alpha x_i \partial_\beta x_i = \hat{\boldsymbol{e}}_\alpha \cdot \hat{\boldsymbol{e}}_\beta \tag{A6}$$

Its inverse $g^{\alpha\beta}$ is given by

$$g^{\alpha\beta} = \text{cofactor } (g_{\alpha\beta})/g \tag{A7}$$

when we adopt the usual notational convention that

$$g = \det(g_{\alpha\beta}) = |\hat{\boldsymbol{e}}_1 \times \hat{\boldsymbol{e}}_2|^2 \tag{A8}$$

It follows that

$$g^{\alpha\beta}g_{\beta\gamma} = \delta^\alpha_\gamma \tag{A9}$$

Consider now a vector field $\boldsymbol{u}$ embedded on the

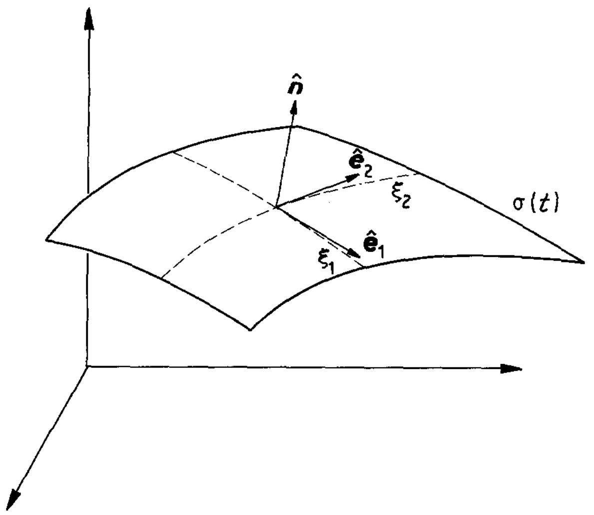

Figure 4 Definition of the curvilinear coordinate system for the surface $\sigma(t)$.

surface $\sigma(t)$. This field, having only components directed along the surface basis vectors $\hat{e}_\alpha$, can be written as

$$\boldsymbol{u} = u^\alpha \hat{e}_\alpha = u_\alpha \hat{e}^\alpha \tag{A10}$$

with either contravariant components u^α or covariant components u_α. The basis vectors having raised Greek indices are by definition related to those with lowered indices through the metric tensor

$$\hat{e}^\alpha = g^{\alpha\beta}\hat{e}_\beta \tag{A11}$$

and so accordingly

$$u^\alpha = g^{\alpha\beta}u_\beta \quad u_\alpha = g_{\alpha\beta}u^\beta \tag{A12}$$

The unit vector $\hat{n}$ normal to the surface $\sigma(t)$ is obtained from the contravariant basis vectors through the relation

$$\hat{n}(\xi^\alpha, t) = (\hat{e}_1 \times \hat{e}_2)/|\hat{e}_1 \times \hat{e}_2|, \tag{A13}$$

or equivalently,

$$n_i = \tfrac{1}{2}e^{\alpha\beta}\varepsilon_{ijk}\partial_\alpha x_j \partial_\beta x_k, \tag{A14}$$

which makes use of the completely antisymmetric tensor ε_{ijk}. The surface tensor $e^{\alpha\beta}$ appearing in this expression is given as

$$e^{\alpha\beta} = \varepsilon^{\alpha\beta}/\sqrt{g} \quad e_{\alpha\beta} = \varepsilon_{\alpha\beta}\sqrt{g} \tag{A15}$$

where

$$\varepsilon^{11} = \varepsilon^{22} = \varepsilon_{11} = \varepsilon_{22} = 0 \tag{A16}$$

$$\varepsilon^{12} = -\varepsilon^{21} = \varepsilon_{12} = -\varepsilon_{21} = 1 \tag{A17}$$

One finds that

$$e^{\alpha\beta}e_{\beta\gamma} = \delta^\alpha_\gamma \tag{A18}$$

so that the basis vectors relevant to the surface obey the identities

$$\hat{n}\cdot\hat{n} = 1 \quad \hat{n}\cdot\hat{e}_\alpha = 0 \tag{A19}$$

$$\hat{e}_\alpha \times \hat{e}_\beta = e_{\alpha\beta}\hat{n} \quad \hat{n}\times\hat{e}_\alpha = g_{\alpha\beta}e^{\beta\gamma}\hat{e}_\gamma \tag{A20}$$

A result of particular importance to the subsequent discussion can now be introduced provided we make the observation that

$$g^{\alpha\beta} = e^{\alpha\gamma}e^{\beta\delta}g_{\gamma\delta} \tag{A21}$$

This is so because the antisymmetric property of the surface tensors performs the usual task of inverting a 2×2 matrix by switching the diagonals and negating the off-diagonal entries. The additional requirement that one divides by the determinant is accounted for by the appropriate factors of $\sqrt{g}$. In a perhaps lengthy but nonetheless straightforward way one can then show that

$$g^{\alpha\beta}\hat{e}_{\alpha_i}\hat{e}_{\beta_j} = g^{\alpha\beta}\partial_\alpha x_i \partial_\beta x_j = \delta_{ij} - n_i n_j \tag{A22}$$

by utilizing the complete expression for $\hat{n}$ in the right-hand side of the above equation and reexpressing the antisymmetric tensors as

$$\varepsilon_{ikm}\varepsilon_{jln} = \det\begin{vmatrix} \delta_{ij} & \delta_{j} & \delta_{mj} \\ \delta_{il} & \delta_{kl} & \delta_{ml} \\ \delta_{in} & \delta_{kn} & \delta_{mn} \end{vmatrix} \tag{A23}$$

Reference to Equation A22 will later be made in a digression concerning the rays traced out by the time development of the wavefront.

Turning now our attention to the changes arising in various quantities during displacements along the surface, we are led to consider the derivatives of the basis vectors with respect to the curvilinear coordinates ξ_β. We write

$$\partial_\beta \hat{e}_\alpha = \Gamma^\gamma_{\alpha\beta}\hat{e}_\gamma + \Gamma^n_{\alpha\beta}\hat{n}, \tag{A24}$$

thus introducing the Christoffel symbols as projections of $\partial_\beta\hat{e}_\alpha$ along the basis vectors. From the orthogonality conditions A19 and A20 we have

$$\Gamma^\gamma_{\alpha\beta} = \hat{e}^\gamma \cdot \partial_\beta\hat{e}_\alpha \quad \Gamma^n_{\alpha\beta} = \hat{n}\cdot\partial_\beta\hat{e}_\alpha \tag{A25}$$

By repeated reference to Equation A6 for various permutations of indices, the first of these expressions above can be used to show that

$$\Gamma^\gamma_{\alpha\beta} = g^{\gamma\delta}\hat{e}_\delta\cdot\partial_\beta\hat{e}_\alpha = \tfrac{1}{2}g^{\gamma\delta}(\partial_\beta g_{\alpha\delta} + \partial_\alpha g_{\beta\delta} - \partial_\delta g_{\alpha\beta}) \tag{A26}$$

from whence it follows that

$$\Gamma^\alpha_{\alpha\beta} = \tfrac{1}{2}g^{\alpha\delta}\partial_\beta(g_{\alpha\delta}) = \tfrac{1}{2}\partial_\beta(\ln g) \tag{A27}$$

Use was made of the result

$$\partial_\beta(g^{\alpha\delta}g_{\alpha\delta}) = \partial_\beta(e^{\alpha\gamma}e^{\delta\varepsilon}g_{\gamma\varepsilon}g_{\alpha\delta}) = 0 \tag{A28}$$

Equation A27 is vital for the following important result involving displacement changes of the surface normal.

With reference to Equation A14, the derivative of the unit vector $\hat{n}$ with respect to $\xi\gamma$ takes the form

$$\partial_\gamma n_i = \partial_\gamma(\tfrac{1}{2}e^{\alpha\beta}\varepsilon_{ijk}\partial_\alpha x_j\partial_\beta x_k) \tag{A29}$$

$$= -\tfrac{1}{2}\partial_\gamma(\ln g)\,n_i + e^{\alpha\beta}\varepsilon_{ijk}\partial_\gamma(\partial_\alpha x_j)\,\partial_\beta x_k \tag{A30}$$

where the antisymmetry of both $e^{\alpha\beta}$ and ε_{ijk} have been exploited to combine two similar terms arising from Equation A29. Using the Christoffel form of $\partial_\gamma\hat{e}_\alpha$ and Equation A20, this expression becomes

$$\partial_\gamma n_i = -\tfrac{1}{2}\partial_\gamma(\ln g)\,n_i + e^{\alpha\beta}\Gamma^\delta_{\alpha\gamma}e_{\delta\beta}n_i - e^{\alpha\beta}\Gamma^n_{\alpha\gamma}e^{\delta\varepsilon}g_{\beta\delta}\partial_\varepsilon x_i \tag{A31}$$

$$= -g^{\alpha\varepsilon}\Gamma^n_{\alpha\gamma}\partial_\varepsilon x_i \tag{A32}$$

having cancelled the first and second terms. This expression will be found to be significant for the discussion in the next section.

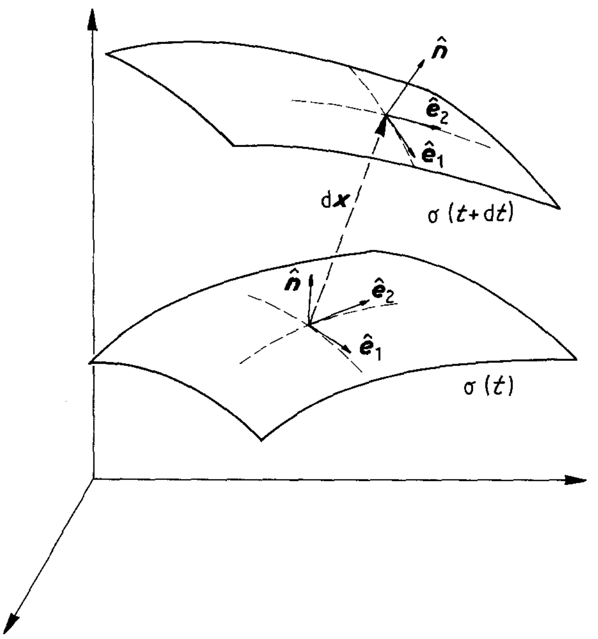

Figure 5 Time development of the curvilinear coordinate system on $\sigma(t)$ along the trajectory $\mathrm{d}\boldsymbol{x}$.

Appendix B: Ray equations

We now extend the scope of our analysis to include the time development of the surface $\sigma(t)$ and its associated mathematical quantities – see Fig. 5. Note, for a given parametrization of $\sigma(t)$, that a point $\boldsymbol{x}(t)$ having its motion confined to the surface must be given by the form

$$x_i = x_i(\xi^\alpha(t), t) \tag{A33}$$

so that the velocity along this ray necessarily becomes

$$u_i = \frac{\mathrm{d}x_i}{\mathrm{d}t} = \frac{\partial x_i}{\partial t} + \frac{\partial x_i}{\partial \xi^\alpha}\frac{\partial \xi^\alpha}{\partial t} \tag{A34}$$

$$\equiv \partial_t x_i + \hat{e}_{\alpha_i}\partial_t \xi^\alpha \tag{A35}$$

Recalling the form of Equation A10, the vector $\boldsymbol{u}$ can equivalently be given by

$$\boldsymbol{u} = u^\alpha \hat{\boldsymbol{e}}_\alpha + u^n \hat{\boldsymbol{n}} \tag{A36}$$

so that the normal component of the velocity is then

$$u^n = \boldsymbol{u}\cdot\hat{\boldsymbol{n}} = \partial_t \boldsymbol{x}\cdot\hat{\boldsymbol{n}} \tag{A37}$$

This component, being just the normal propagation velocity of the wavefront, is independent of the parametrization of the surface and is aptly called the phase velocity of the front.

If we consider the form of the variation of u^n for an infinitessimal displacement along the surface, we have

$$\partial_\alpha u^n = \partial_\alpha(\partial_t x_i n_i) \tag{A38}$$

$$= -\partial_\alpha x_i \partial_t n_i + \partial_t x_i \partial_\alpha n_i \tag{A39}$$

where use has been made of the result that $(\partial_\alpha x_i) n_i = 0$. Equation A39 is multiplied by $g^{\alpha\beta}\partial_\beta x_j$ to obtain

$$g^{\alpha\beta}\partial_\alpha u^n \partial_\beta x_j = -g^{\alpha\beta}\partial_\alpha x_i \partial_\beta x_j \partial_t n_i + \partial_t x_i g^{\alpha\beta}\partial_\alpha n_i \partial_\beta x_j \tag{A40}$$

which, by using Equations A22 and A32 reduces to

$$g^{\alpha\beta}\partial_\alpha u^n \partial_\beta x_j = -(\delta_{ij} - n_i n_j)\partial_t n_i - \partial_t x_i g^{\alpha\beta} g^{\gamma\beta}\Gamma^n_{\gamma\alpha}\partial_\delta x_i \partial_\beta x_j \tag{A41}$$

However, $n_i \cdot \partial_t n_i = 0$, and, from Equations A35 and A36

$$\partial_t x_i \partial_\delta x_i = u_i \partial_\delta x_i - g_{\alpha\delta}\partial_t \xi^\alpha \tag{A42}$$

$$= g_{\alpha\delta} u^\alpha - g_{\alpha\delta}\partial_t \xi^\alpha \tag{A43}$$

so we have that

$$g^{\alpha\beta}\partial_\alpha u^n \partial_\beta x_j = -\delta_{ij}\partial_t n_i - g^{\alpha\beta}\Gamma^n_{\gamma\alpha}\partial_\beta x_j(u^\gamma - \partial_t \xi^\gamma) \tag{A44}$$

Hence, the partial time derivative of n_i is

$$\partial_t n_i = -g^{\alpha\beta}\partial_\alpha u^n \partial_\beta x_i - g^{\alpha\beta}\Gamma^n_{\gamma\alpha}\partial_\beta x_i(u^\gamma - \partial_t \xi^\gamma) \tag{A45}$$

and the total time derivative is

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = \frac{\partial n_i}{\partial t} + \frac{\partial n_i}{\partial \xi^\alpha}\frac{\partial \xi^\alpha}{\partial t} \tag{A46}$$

$$= \partial_t n_i - g^{\alpha\beta}\Gamma^n_{\gamma\alpha}\partial_\beta x_i \partial_t \xi^\alpha \tag{A47}$$

$$= -g^{\alpha\beta}\partial_\alpha u^n \partial_\beta x_i - g^{\alpha\beta}\Gamma^n_{\gamma\alpha}\partial_\beta x_i u^\gamma \tag{A48}$$

This is the total time rate of change of the surface normal along the ray trajectory A33 having a velocity A35 and A36.

If the trajectory is chosen to follow the normal to the surface, that is $u\gamma = 0$, ($\gamma = 1, 2$), then the rate of change of $\hat{\boldsymbol{n}}$ becomes

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = -g^{\alpha\beta}\partial_\alpha u^n \partial_\beta x_i \tag{A49}$$

$$= -(\delta_{ij} - n_i n_j)\frac{\partial u^n}{\partial x_j} \tag{A50}$$

when

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = u^n n_i \tag{A51}$$

Equation A50 is obtained by transforming to spatial coordinates using the relation

$$\partial_\alpha u^n = \frac{\partial u^n}{\partial x_j}\frac{\partial x_j}{\partial \xi^\alpha} \tag{A52}$$

The coupled ray equations A50 and A51 describe the trajectories directed along the phase velocity of a moving wavefront and are in agreement with those given by Eringen and Suhubi for the displacement derivative of $\hat{\boldsymbol{n}}$.

Of interest to us, however, is the case in which the trajectory follows not the phase velocity vector of the wavefront, but the *group velocity* vector. In this case, we substitute the terms in Equation A48 involving $\boldsymbol{u}$ for those involving $\boldsymbol{c}$, where

$$c_i = \frac{\partial u^n}{\partial n_i} \quad c_i n_i = u^n \tag{A53}$$

We obtain

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = -g^{\alpha\beta}\partial_\alpha u^n \partial_\beta x_i - g^{\alpha\beta}\Gamma^n_{\gamma\alpha}\partial_\beta x_i c^\gamma \tag{A54}$$

which, by making use of the change of variable $u^n(\xi^\alpha) = u^n[n_j(\xi^\alpha)]$, becomes

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = -g^{\alpha\beta}c_j\partial_\alpha n_j \partial_\beta x_i - g^{\alpha\beta}\Gamma^n_{\gamma\alpha}\partial_\beta x_i \boldsymbol{c}\cdot\hat{\boldsymbol{e}}^\gamma \tag{A55}$$

$$= g^{\alpha\beta}g^{\gamma\beta}\Gamma^n_{\gamma\alpha}(\boldsymbol{c}\cdot\hat{\boldsymbol{e}}_\delta \partial_\beta x_i - \partial_\beta x_i \boldsymbol{c}\cdot\hat{\boldsymbol{e}}_\delta) = 0 \tag{A56}$$

In conclusion, we find for the ray trajectories following the group velocity of a wavefront, that the components of the surface normal remain constant. The ray then must trace out a straight line since the velocity being only a function of the components n_i will remain constant in magnitude and direction along such a trajectory.

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