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ABSTRACT

An anisotropic constitutive relation has been incorporated into the Lagrangian finite-difference wavecode TOODY. This report contains the details of the implementation of the constitutive relation in the wavecode and an example of its use.

1. Introduction

Finite difference wave propagation codes solve the finite-difference analogs to the partial differential equations expressing the conservation laws of continuum mechanics. In addition to these conservation laws, constitutive equations must be supplied which characterize the physical properties of the materials involved. The simplest constitutive models assume the material to be hydrodynamic and supply a pressure-volume relationship. More sophisticated models include complete thermodynamic potentials and allow such phenomena as phase transitions, but still involve only the pressure and volume. Further refinement introduces the complete stress and strain tensors but assumes the materials to be isotropic. However, many materials may be very poorly described by isotropic calculations, and thus anisotropic material models become necessary.

The anisotropic constitutive equation presented here uses the general formalism of anisotropic elasticity to relate each stress component to all of the strain components through the tensor of elastic stiffness coefficients. Third-order elastic stiffness coefficients are also included to allow for non-linear effects. However, much room is left for refinement. The coefficients are assumed to be constant, and there is no explicit energy dependence. The model could be improved by introducing a complete thermodynamic treatment. However, for most anisotropic materials the information does not presently exist to allow a complete thermodynamic description, and thus the inclusion of the formalism in the code would not be worthwhile at this time. The most useful improvement to the present model would be the addition of plasticity to the formulation.

It should be noted that the constitutive model is cast in a fully three-dimensional form with complete freedom of specification of all of the independent elastic constants. However, it has been incorporated into the two-dimensional Lagrangian wavecode TOODY[1]. Since the response of an anisotropic material will generally be three-dimensional, care must be taken in the use of this model in TOODY and other two-dimensional codes to ensure that the physical situation being calculated is actually two-dimensional.

2. Anisotropic Constitutive Relation

Let the vector $\vec{x}$ be the position at time t of the particle which was at position $\vec{X}$ at time t = 0. Thus

$$\vec{x} = \vec{x}(\vec{X},t) \ , \tag{1}$$

where $\vec{X}$ is the material, or Lagrangian, coordinate (defined here as the position at time t = 0), and $\vec{x}$ is the spatial or Eulerian coordinate. Equation (1) can be viewed as a transformation from $\vec{X}$ to $\vec{x}$ at time t. The transformation matrix for this transformation is called the material deformation gradient and its components are given by

$$F_{ij} = \frac{\partial x_i}{\partial X_j} \ . \tag{2}$$

The determinant of the matrix $\underline{F}$ is called the Jacobian, J, and is related to the density, ρ, by

$$J = \rho_o/\rho \tag{3}$$

where ρ_o is the density in the reference configuration. The Lagrange-Green finite strain may be related to $\underline{F}$ by[2]

$$\underline{L} = \frac{1}{2}\left(\underline{F}^T\underline{F} - \underline{I}\right) \ , \tag{4}$$

where $\underline{I}$ is the identity matrix. In index notation this becomes*

$$L_{ij} = \frac{1}{2}\left(\frac{\partial x_k}{\partial X_i}\frac{\partial x_k}{\partial X_j} - \delta_{ij}\right) \ . \tag{5}$$

Here $\underline{L}$ has been taken negative in compression and δ_{ij} is the Kronecker delta.

The nth order adiabatic elastic stiffness coefficients may be defined by[3]

$$C_{ijk\ell mp\ldots} = \rho_o\left(\frac{\partial^n \mathcal{E}}{\partial L_{ij}\,\partial L_{k\ell}\,\partial L_{mp}\cdots}\right)_s \ , \tag{6}$$

where $\mathcal{E}$ is the specific internal energy, or internal energy per unit mass, and the

*Repeated subscripts imply summation.

subscript s implies differentiation at constant entropy. The series expansion of $\mathcal{E}$ about a state of zero strain is[4]

$$\rho_o \mathcal{E} = \frac{1}{2} C_{ijk\ell} L_{ij} L_{k\ell} + \frac{1}{6} C_{ijk\ell mn} L_{ij} L_{k\ell} L_{mn} + \dots , \tag{7}$$

where the $C_{ijk\ell}$ are the regular, or second order constants, and the $C_{ijk\ell mn}$ are the third-order constants.* The stress is related to the internal energy by[5]

$$\Sigma_{ij} = \rho_o \left(\frac{\partial \mathcal{E}}{\partial L_{ij}} \right)_s \tag{8}$$

where $\underset{\sim}{\Sigma}$ is the second Piola-Kirchoff stress tensor, which is related to the Cauchy stress $\underset{\sim}{\sigma}$ by[2]

$$\underset{\sim}{\sigma} = \frac{1}{J} \underset{\sim}{F} \underset{\sim}{\Sigma} \underset{\sim}{F}^T \quad . \tag{9}$$

Thus, from Equations (7) and (8),

$$\begin{aligned} \Sigma_{ij} &= \frac{\partial}{\partial L_{ij}} \left(\frac{1}{2} C_{k\ell mn} L_{k\ell} L_{mn} + \frac{1}{6} C_{k\ell mnpq} L_{k\ell} L_{mn} L_{pq} \right) \\ &= \frac{1}{2} C_{ijmn} L_{mn} + \frac{1}{2} C_{k\ell ij} L_{k\ell} + \frac{1}{6} C_{ijmnpq} L_{mn} L_{pq} \\ &\quad + \frac{1}{6} C_{k\ell ijpq} L_{k\ell} L_{pq} + \frac{1}{6} C_{k\ell mnij} L_{k\ell} L_{mn} , \end{aligned} \tag{10}$$

where the fact that

$$\frac{\partial L_{ij}}{\partial L_{k\ell}} = \delta_{ik} \delta_{j\ell} \tag{11}$$

has been used.

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*The $C_{ijk\ell}$ form a fourth-order tensor, and the $C_{ijk\ell mn}$ constitute a sixth-order tensor. The definition of an nth order tensor is that it transforms under orthognal transformation by the rule

$$B'_{ijk\ell \dots} = a_{ip} a_{jq} a_{kr} a_{\ell s} \dots B_{pqrs \dots}$$

where the a_{ij} are the components of the transformation matrix.

Now from Equation (6), the elastic stiffness coefficients are symmetric with respect to the exchange of pairs of indices. since

$$C_{ijk\ell mn} = \rho_o \left(\frac{\partial^3 \mathcal{E}}{\partial L_{ij} \partial L_{k\ell} \partial L_{mn}} \right)_s = \left(\frac{\partial^3 \mathcal{E}}{\partial L_{k\ell} \partial L_{ij} \partial L_{mn}} \right)_s = C_{k\ell ijmn} \quad . \tag{12}$$

Using this fact, Equation (10) becomes

$$\Sigma_{ij} = C_{ijk\ell} L_{k\ell} + \frac{1}{2} C_{ijk\ell mn} L_{k\ell} L_{mn} \quad . \tag{13}$$

Equations (5) and (13) provide the constitutive relation describing anisotropic elasticity, including third-order constants. The constitutive relation must satisfy the law of objectivity.[2,6] This states that the constitutive relation must be independent of the observer, and thus must be invariant under translations and rotations of the coordinate system. It is shown in Reference 6 that both $\underset{\sim}{\Sigma}$ and $\underset{\sim}{L}$ are frame-invariant with respect to rotations of the Eulerian coordinate system. That is, their components are not affected by such rotations. They are frame-indifferent with respect to rotations of the Lagrangian coordinate system, which means that they transform under the normal tensor transformation rule for orthogonal transformations of the Lagrangian coordinate system. Thus, Equation (13) satisfies the law of objectivity. Physically, this is due to the fact that all components of Equation (13) are defined with respect to the Lagrangian coordinate system and are unaffected by material rotation with respect to the Eulerian system. However, the equations of motion in most codes are written with respect to the Eulerian system and thus require the Cauchy stress $\underset{\sim}{\sigma}$. This can be obtained from the second Piola-Kirchoff stress using Equation (9), which in index notation becomes

$$\sigma_{ij} = \frac{1}{J} F_{ik} F_{j\ell} \Sigma_{k\ell} \quad . \tag{14}$$

Thus, Equations (5), (13) and (14) define a frame-indifferent anisotropic constitutive relation suitable for use in wavecodes.

3. Reduced Notation

There are 9 components in the stress and strain tensors, 81 second-order elastic constants, and 729 third-order elastic constants. However, the stress and strain tensors are symmetric, reducing the number of independent components to 6. The elastic constants, as shown in Equation (12), are symmetric with respect to the exchange of pairs of indices. They are also symmetric with respect to interchange of indices within a pair, as can be seen by considering Equation (12) in the context of the symmetry of L. This reduces the number of independent second-order elastic components to 21, and the number of independent third-order elastic constants to 56.

Because of these symmetries, it would be very wasteful computationally to perform calculations with the constitutive relation in the form given by Equation (13). The situation can be improved by introducing a reduced notation which replaces each pair of indices by a single index. The convention is as follows:

Double Subscript	Single Subscript
11	1
22	2
33	3
23 or 32	4
13 or 31	5
12 or 21	6

The convention carries directly through for the stresses, but factors of two must be introduced for strains with index greater than or equal to 4. Thus:

$$\Sigma_1 = \Sigma_{11}$$
$$\Sigma_2 = \Sigma_{22}$$
$$\Sigma_3 = \Sigma_{33}$$
$$\Sigma_4 = \Sigma_{23} = \Sigma_{32}$$
$$\Sigma_5 = \Sigma_{13} = \Sigma_{31}$$
$$\Sigma_6 = \Sigma_{12} = \Sigma_{21}$$
$$L_1 = L_{11}$$

$$L_2 = L_{22}$$
$$L_3 = L_{33}$$
$$L_4 = 2L_{23} = 2L_{32}$$
$$L_5 = 2L_{13} = 2L_{31}$$
$$L_6 = 2L_{12} = 2L_{21} \ .$$

The notation holds directly for the elastic constants, with each pair of subscripts being replaced by a single subscript. Thus:

$$C_{14} = C_{1123} = C_{1132}$$
$$C_{235} = C_{223313} = C_{223331} \text{ etc.}$$

Using this convention, Equation (13) becomes*

$$\Sigma_\lambda = C_{\lambda\mu}L_\mu + \frac{1}{2} C_{\lambda\mu\nu}L_\mu L_\nu \ . \tag{15}$$

The elastic constants in the reduced notation are symmetric with respect to any permutation of the indices. However, Equation (15) involves considerably less computation since there are now summations over 36 second-order and 216 third-order constants, of which 21 and 56, respectively, are independent.

A relationship may be derived which allows the elastic constant tensors to be transformed under rotation in the reduced notation directly rather than converting to the double index notation. The transformation rule for a second-order tensor is

$$B'_{ij} = a_{ik}a_{j\ell}B_{k\ell} \ , \tag{16}$$

where the a_{ij} are the components of the transformation matrix. A matrix $\underline{A}$ may be defined which will allow Equation (16) to be written in reduced notation as:

$$B'_\lambda = A_{\lambda\mu}B_\mu \ . \tag{17}$$

$\underline{A}$ may be defined by noticing that Equation (16) may be written

$$B'_{ij} = a_{ik}a_{j\ell}B_{k\ell}\delta_{k\ell} + \sum_{\ell=1}^{3}\sum_{k=1}^{\ell-1}(a_{ik}a_{j\ell} + a_{i\ell}a_{jk})B_{k\ell} \ , \tag{18}$$

*Greek subscripts will be used to denote summation using the reduced notation.

where the symmetry of $\underset{\sim}{B}$ has been assumed. The first term contains components of $\underset{\sim}{B}$ which correspond to the single indices 1, 2, and 3, while the second contains components which correspond to single indices 4, 5, and 6. Thus, if λ corresponds to ij and μ corresponds to $k\ell$, $\underset{\sim}{A}$ is defined by

$$A_{\lambda\mu} = a_{ik}a_{j\ell} \ , \tag{19}$$

for $\mu = 1, 2, 3$ corresponding to $k\ell = 11, 22, 33$, respectively, and

$$A_{\lambda\mu} = a_{ik}a_{j\ell} + a_{i\ell}a_{jk} \ , \tag{20}$$

for $\mu = 4,5,6$ corresponding to $k\ell = 23$ or 32, 13 or 31, 12 or 21, respectively. With Equations (19) and (20) defining $\underset{\sim}{A}$, Equations (16) and (17) are equivalent. The full matrix $\underset{\sim}{A}$ is

$$A = \begin{pmatrix} a_{11}a_{11} & a_{12}a_{12} & a_{13}a_{13} & 2a_{12}a_{13} & 2a_{11}a_{13} & 2a_{11}a_{12} \\ a_{21}a_{21} & a_{22}a_{22} & a_{23}a_{23} & 2a_{22}a_{23} & 2a_{21}a_{23} & 2a_{21}a_{22} \\ a_{31}a_{31} & a_{32}a_{32} & a_{33}a_{33} & 2a_{32}a_{33} & 2a_{31}a_{33} & 2a_{31}a_{32} \\ a_{21}a_{32} & a_{22}a_{32} & a_{23}a_{33} & a_{22}a_{33}+a_{23}a_{32} & a_{21}a_{33}+a_{23}a_{31} & a_{21}a_{32}+a_{22}a_{31} \\ a_{11}a_{31} & a_{12}a_{32} & a_{13}a_{33} & a_{12}a_{33}+a_{13}a_{32} & a_{11}a_{33}+a_{13}a_{31} & a_{11}a_{32}+a_{12}a_{31} \\ a_{11}a_{21} & a_{12}a_{22} & a_{13}a_{23} & a_{12}a_{23}+a_{13}a_{22} & a_{11}a_{23}+a_{13}a_{21} & a_{11}a_{22}+a_{12}a_{21} \end{pmatrix} . \tag{21}$$

Fourth-order tensors transform as follows:

$$B'_{ijk\ell} = a_{iq}a_{jr}a_{ks}a_{\ell t}B_{qrst} \ ; \tag{22}$$

but if $\lambda \leftrightarrow ij$, $\mu \leftrightarrow k\ell$, $\nu \leftrightarrow qr$, and $\phi \leftrightarrow st$, we have*

$$a_{iq}a_{jr}B_{qrst} = A_{\lambda\nu}B_{\nu st} \ , \tag{23}$$

so

$$B'_{\lambda k\ell} = A_{\lambda\nu}a_{ks}a_{\ell t}B_{\nu st} \ . \tag{24}$$

---

*$B_{\nu st}$ has had the reduced notation applied to the first pair of indices but not the second. Thus, $B_{\nu st} = B_{qrst}$ where ν corresponds to qr in the usual reduced rotation convention.

But

$$a_{ks}a_{\ell t}B_{\nu st} = A_{\mu\phi}B_{\nu\phi} \quad . \tag{25}$$

Thus

$$B'_{\lambda\mu} = A_{\lambda\nu}A_{\mu\phi}B_{\nu\phi} \quad . \tag{26}$$

Thus, with $\underset{\sim}{A}$ defined in Equation (21) the general transformation rule for n^{th}-order symmetric tensors may be written in the reduced notation as

$$B'_{\lambda\mu\nu\cdots} = A_{\lambda\phi}A_{\mu\theta}A_{\nu\Psi}\cdots B_{\phi\theta\Psi\cdots} \quad . \tag{27}$$

Equation (27) may be used to transform the elastic constant tensors so that the anisotropic materials are oriented as desired with respect to the Lagrangian frame used in the wavecode calculation.

4. Incorporation into the Wavecode TOODY

The coordinate system used in TOODY is shown in Figure 1.

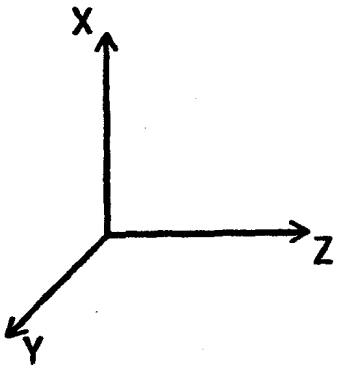

Figure 1. TOODY Coordinate System

The motion occurs in the z,x plane. The convention adopted here will be to equate the z axis with the x_1 axis, x with x_2, and y with x_3. Thus a vector will have components

$$\vec{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} v_z \\ v_x \\ v_y \end{pmatrix}, \tag{28}$$

and a second-order tensor will have components

$$\underset{\sim}{B} = \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix} = \begin{pmatrix} B_{zz} & B_{zx} & B_{zy} \\ B_{xz} & B_{xx} & B_{xy} \\ B_{yz} & B_{yx} & B_{yy} \end{pmatrix}. \tag{29}$$

This allows a standard x_1, x_2, x_3 coordinate system convention to be used, with a permuted naming of the axes when referring to TOODY.

Let a Langrangian position vector be denoted

$$\vec{X} = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} = \begin{pmatrix} Z \\ X \\ Y \end{pmatrix}, \tag{30}$$

and an Eulerian vector be denoted

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} z \\ x \\ y \end{pmatrix} . \tag{31}$$

The deformation gradient is

$$F_{ij} = \frac{\partial x_i}{\partial X_j} \tag{32}$$

TOODY is a two-dimensional code with motion only in the $x_1 x_2$ plane, so the deformation gradient becomes

$$\underset{\sim}{F} = \begin{pmatrix} F_{11} & F_{12} & 0 \\ F_{21} & F_{22} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{\partial z}{\partial Z} & \frac{\partial z}{\partial X} & 0 \\ \frac{\partial x}{\partial Z} & \frac{\partial x}{\partial X} & 0 \\ 0 & 0 & 1 \end{pmatrix} . \tag{33}$$

$\underset{\sim}{F}$ is not symmetric, so the reduced notation does not apply. The Lagrange-Green finite strain is given by Equation (4), which results in

$$\underset{\sim}{L} = \frac{1}{2} \begin{pmatrix} F_{11}^2 + F_{21}^2 - 1 & F_{11}F_{12} + F_{21}F_{22} & 0 \\ F_{11}F_{12} + F_{21}F_{22} & F_{12}^2 + F_{22}^2 - 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} . \tag{34}$$

Thus the strain components in the reduced notation are

$$\underset{\sim}{L} = \begin{pmatrix} L_1 \\ L_2 \\ L_3 \\ L_4 \\ L_5 \\ L_6 \end{pmatrix} = \begin{pmatrix} \frac{1}{2}\left(F_{11}^2 + F_{21}^2 - 1\right) \\ \frac{1}{2}\left(F_{12}^2 + F_{22}^2 - 1\right) \\ 0 \\ 0 \\ 0 \\ F_{11}F_{12} + F_{21}F_{22} \end{pmatrix} . \tag{35}$$

The components of the second Piola-Kirchoff stress in the reduced notation are given

by Equation (15). The components of this stress tensor in terms of the components in the reduced notation are

$$\underset{\sim}{\Sigma} = \begin{pmatrix} \Sigma_1 & \Sigma_6 & \Sigma_5 \\ \Sigma_6 & \Sigma_2 & \Sigma_4 \\ \Sigma_5 & \Sigma_4 & \Sigma_3 \end{pmatrix} . \tag{36}$$

The Cauchy stress is then calculated from Equation (9), which results in the following Cauchy stress components for use in the TOODY equations of motion:

$$\begin{aligned} \sigma_{zz} &= \sigma_{11} = \rho/\rho_o(F_{11}{}^2\Sigma_1 + 2F_{11}F_{12}\Sigma_6 + F_{12}{}^2\Sigma_2) \\ \sigma_{xx} &= \sigma_{22} = \rho/\rho_o(F_{21}{}^2\Sigma_1 + 2F_{21}F_{22}\Sigma_6 + F_{22}{}^2\Sigma_2) \\ \sigma_{zx} &= \sigma_{12} = \rho/\rho_o[F_{11}(F_{21}\Sigma_1 + F_{22}\Sigma_6) + F_{12}(F_{21}\Sigma_6 + F_{22}\Sigma_2)] \\ \sigma_{yy} &= \sigma_{33} = \rho/\rho_o\Sigma_3 \end{aligned} \tag{37}$$

These equations must be finite-differenced to fit into the TOODY difference scheme. Since the stresses are required at time n+1 in TOODY[1] and no rates are involved in the constitutive relation, all quantities are evaluated at time n+1. The only further requirement is a finite-difference expression for the components of the deformation gradient in Equation (33).

Finite-difference approximations to partial derivatives in TOODY are given by[1]

$$\frac{\partial\Psi}{\partial x} = \frac{-1}{A}\oint_C \Psi dz \tag{38}$$

$$\frac{\partial\Psi}{\partial z} = \frac{1}{A}\oint_C \Psi dx , \tag{39}$$

where C is a closed curve over which the line integral is evaluated, and A is the area enclosed by the curve. A portion of the TOODY finite-difference mesh is shown in Figure 2.

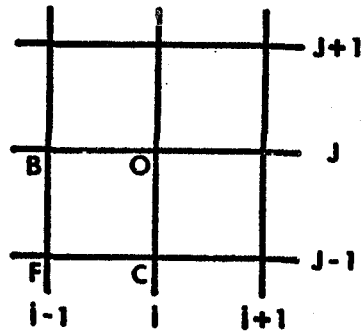

Figure 2. TOODY Finite-Difference Mesh

The integration for the mesh with index i,j is taken over the curve OBFC. Thus,

$$F_{11} = F_{zz} = \frac{\partial z}{\partial Z} = \frac{1}{A_L} \oint z dX \ , \tag{40}$$

where A_L is the area enclosed by curve OBFC in Lagrangian coordinates. Taking z to be constant along each of the line segments and equal to the average of the values at the endpoints, this becomes

$$F_{11} = \frac{1}{2A_L} [(z_\theta - z_F)(X_B - X_C) + (z_C - z_B)(X_\theta - X_F)] \ . \tag{41}$$

Similarly

$$F_{12} = \frac{\partial z}{\partial X} = \frac{1}{2A_L} [(z_\theta - z_F)(Z_C - Z_B) + (z_B - z_C)(Z_\theta - Z_F)] \tag{42}$$

$$F_{21} = \frac{\partial x}{\partial Z} = \frac{1}{2A_L} [(x_\theta - x_F)(X_B - X_C) + (x_C - x_B)(X_\theta - X_F)] \tag{43}$$

$$F_{22} = \frac{\partial x}{\partial X} = \frac{1}{2A_L} [(x_\theta - x_F)(Z_C - Z_B) + (x_B - x_C)(Z_\theta - Z_F)] \ . \tag{44}$$

In general, this will require storing the initial positions for every point. However, if the initial mesh is uniform with spacing δL in each direction, then Equations (41) through (44) reduce to

$$F_{11} = \frac{1}{2\delta L} (z_\theta + z_C - z_F - z_B) \tag{45}$$

$$F_{12} = \frac{1}{2\delta L} (z_\theta + z_B - z_F - z_C) \tag{46}$$

$$F_{21} = \frac{1}{2\delta L} (x_\theta + x_C - x_F - x_B) \tag{47}$$

$$F_{22} = \frac{1}{2\delta L} (x_\theta + x_B - x_F - x_C) \ . \tag{48}$$

Equations (45) through (48), (35), (15) and (37) constitute an anisotropic constitutive relation suitable for inclusion in TOODY. If the initial mesh is not uniform, Equations (41) through (44) may be used in place of Equations (45) through (48).

5. Application

An example of the application of this constitutive relation is the calculation of the normal impact of an x-cut quartz plate on a y-cut quartz plate. An analytic solution for this problem excluding the third-order constants has been given by Johnson.[7] He shows that the anisotropy of the crystal produces two coupled longitudinal-shear waves which propagate into the y-cut quartz target. The motion is two-dimensional and thus suitable for TOODY calculations. For the case in which the materials become bonded together at the impact interface, the first wave travels with a velocity of 6.0 km/s and reflection from the free rear surface of the target results in longitudinal and transverse velocity components which are 38% and 79% of the impact velocity, respectively. The second wave has a velocity of 4.3 km/s and a longitudinal free surface velocity component 100% of the impact velocity. The transverse free surface velocity component of the second wave is in the negative x_2 direction and has a magnitude which is 7% of the impact velocity. Results were also obtained for the case of no transverse stresses being transmitted across the impact interface (no friction on interface). Figure 3, taken from reference 7, summarizes the results.

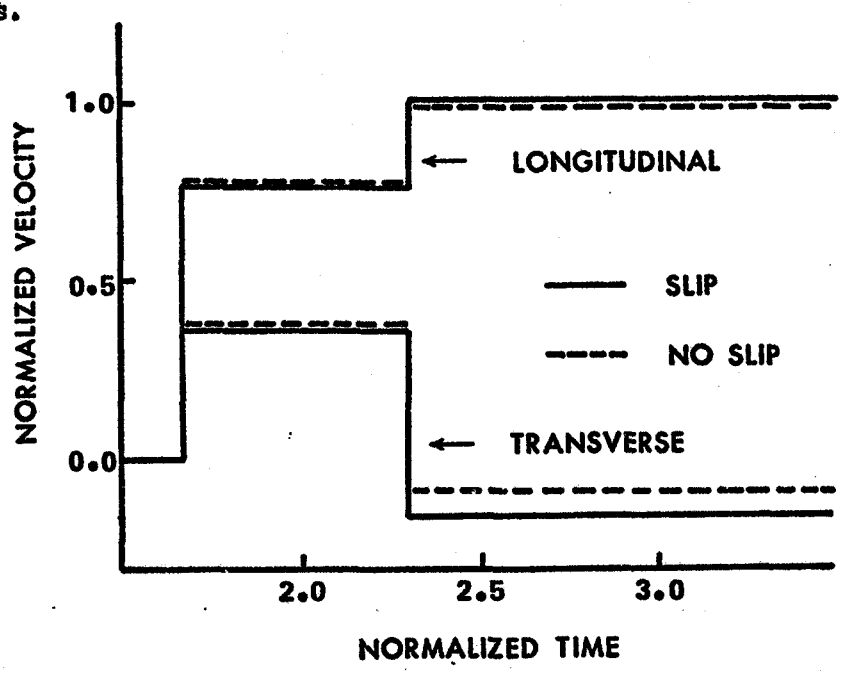

Figure 3. Analytical Results for Longitudinal and Transverse Components of Free Surface Velocity in Impact of x-cut Quartz on y-cut Quartz

The orientation of the crystallographic reference systems relative to the TOODY coordinate system is shown in Figure 4.

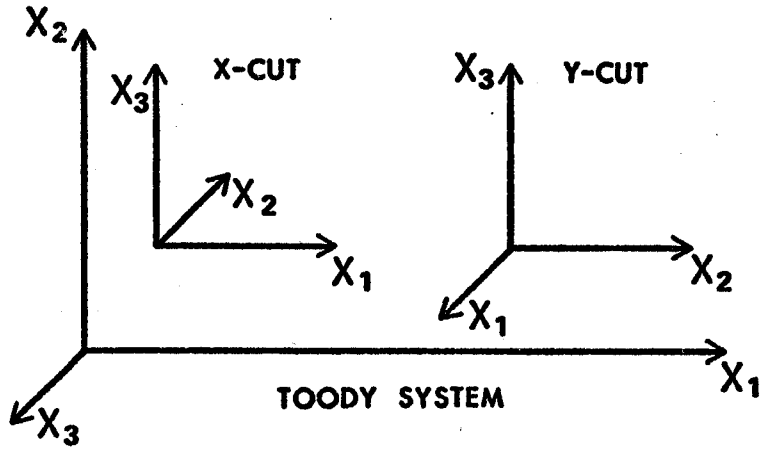

Figure 4. Relation of Crystallographic Axes to TOODY Axes

Thus, for the x-cut quartz, the rotation matrix, defined by Equation (16), is

$$\underset{\sim}{a} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \tag{49}$$

and for the y-cut quartz, it is

$$\underset{\sim}{a} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} . \tag{50}$$

Appendix A contains the input for the constitutive relation, and Appendix B contains the elastic constants for α-quartz.

The calculation used symmetry boundaries so that quantities varied only in the TOODY x_1 direction, and thus zoning was required only in the x_1 dimension. Calculations were performed for various impact velocities. Results for the no-slip case are shown in Table I. The result at very low strains agree with Johnson's results, which describe the acoustic case. The results at higher strains are affected by the

Table I

Summary of Calculational Results for Impact of x-cut Quartz on y-cut Quartz. No Slip at Impact Interface

Impact Velocity (km/sec)	Longitudinal Free Surface Velocity (% of Impact Velocity)		Transverse Free Surface Velocity (% of Impact Velocity)		Wave Speed (km/sec)	
	1st Wave	2nd Wave	1st Wave	2nd Wave	1st Wave	2nd Wave
.0012	78.86	100.75	38.11	-7.12	6.006	4.308
.12	79.68	100.37	38.54	-6.49	5.992	4.401
.22	80.34	100.08	38.91	-6.01	5.980	4.474
.33	81.06	99.80	39.35	-5.52	5.967	4.552

third-order elastic constants, especially for the second wave. This is in agreement with experimental results for longitudinal and transverse free surface velocity components for this configuration which were obtained using a velocity interferometer technique.[8]

6. Conclusions

An anisotropic constitutive relation has been incorporated into the finite-difference wavecode TOODY. The relation has been formulated in complete three-dimensional generality. However, since TOODY is a two-dimensional code, care must be taken to ensure that the physical configuration being calculated is actually one of two-dimensional strain. The model has been applied to a specific configuration and results have been obtained which agree with both analytical and experimental results. The most useful improvement of the model would be the addition of plasticity.

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Appendix A

Input Instructions

The input for the anisotropic constitutive relation consists of the following cards. The numbers in parenthesis following the field are the column numbers in which the variable appears on the card.

Card 1 (5E10.0)

Field	Variable Name	Description
1 (1-10)	ρ_o	Initial density of the material.
2 (11-20)	C_o	Largest sound speed possible in the material.
3 (21-30)	ROTSW	If not equal to zero, the crystallographic axes are not identical with the TOODY axes, and the elastic constant tensor will be rotated.
4 (31-40)	TOSW	If not equal to zero, third-order elastic constants will be used.
5 (41-50)	DL	Initial uniform spacing of the mesh representing the material. (A uniform mesh has been assumed, but this could easily be changed if required.)

Card 2 (8E10.0) Second-Order Elastic Constants

Field	Variable Name	Description
1 (1-10)	C_{11}	Second-Order Elastic Constants
2 (11-20)	C_{12}	
3 (21-30)	C_{13}	
4 (31-40)	C_{14}	
5 (41-50)	C_{15}	

Card 2 (8E10.0) Cont'd

Field	Variable Name	Description
6 (51-60)	C_{16}	Second-Order Elastic Constants
7 (61-70)	C_{22}	
8 (71-80)	C_{23}	

Card 3 (8E10.0) Second-Order Elastic Constants

Field	Variable Name	Description
1 (1-10)	C_{24}	Second-Order Elastic Constants
2 (11-20)	C_{25}	
3 (21-30)	C_{26}	
4 (31-40)	C_{33}	
5 (41-50)	C_{34}	
6 (51-60)	C_{35}	
7 (61-70)	C_{36}	
8 (71-80)	C_{44}	

Card 4 (8E10.0) Second-Order Elastic Constants

Field	Variable Name	Description
1 (1-10)	C_{45}	Second-Order Elastic Constants
2 (11-20)	C_{46}	
3 (21-30)	C_{55}	
4 (31-40)	C_{56}	
5 (41-50)	C_{66}	

Card 4 (8E10.0) Rotation Matrix. Present only if ROTSW $\neq$ 0 on Card 1.

Field	Variable Name	Description
1 (1-10)	a_{11}	Components of rotation matrix as defined in Equation (16).
2 (11-20)	a_{12}	

Card 4 (8E10.0) Cont'd

Field	Variable Name	Description
3 (21-30)	a_{13}	Components of rotation matrix as defined in Equation (16).
4 (31-40)	a_{21}	
5 (41-50)	a_{22}	
6 (51-60)	a_{23}	
7 (61-70)	a_{31}	
8 (71-80)	a_{32}	

Card 5 (E10.0) Rotation Matrix. Present only if ROTSW ≠ 0 on Card 1.

Field	Variable Name	Description
1 (1-10)	a_{33}	Components of rotation matrix as defined in Equation (16).

Card 6 (8E10.0) Third-Order Elastic Constants. Present only if TOSW ≠ 0 on Card 1.

Field	Variable Name	Description
1 (1-10)	C_{111}	Third-Order Elastic Constants
2 (11-20)	C_{112}	
3 (21-30)	C_{113}	
4 (31-40)	C_{114}	
5 (41-50)	C_{115}	
6 (51-60)	C_{116}	
7 (61-70)	C_{122}	
8 (71-80)	C_{123}	

Card 7 (8E10.0) Third-Order Elastic Constants. Present only if TOSW ≠ 0 on Card 1.

Field	Variable Name	Description
1 (1-10)	C_{124}	Third-Order Elastic Constants
2 (11-20)	C_{125}	
3 (21-30)	C_{126}	

Card 7 (8E10.0) Cont'd

Field	Variable Name	Description
4 (31-40)	C_{133}	Third-Order Elastic Constants
5 (41-50)	C_{134}	
6 (51-60)	C_{135}	
7 (61-70)	C_{136}	
8 (71-80)	C_{144}	

Card 8 (8E10.0) Third-Order Elastic Constants. Present only if TOSW ≠ 0 on Card 1.

Field	Variable Name	Description
1 (1-10)	C_{145}	Third-Order Elastic Constants
2 (11-20)	C_{146}	
3 (21-30)	C_{155}	
4 (31-40)	C_{156}	
5 (41-50)	C_{166}	
6 (51-60)	C_{222}	
7 (61-70)	C_{223}	
8 (71-80)	C_{224}	

Card 9 (8E10.0) Third-Order Elastic Constants. Present only if TOSW ≠ 0 on Card 1.

Field	Variable Name	Description
1 (1-10)	C_{225}	Third-Order Elastic Constants
2 (11-20)	C_{226}	
3 (21-30)	C_{233}	
4 (31-40)	C_{234}	
5 (41-50)	C_{235}	
6 (51-60)	C_{236}	
7 (61-70)	C_{244}	
8 (71-80)	C_{245}	

Card 10 (8E10.0) Third-Order Elastic Constants. Present only if TOSW ≠ 0 on Card 1.

Field	Variable Name	Description
1 (1-10)	C_{246}	Third-Order Elastic Constants
2 (11-20)	C_{255}	
3 (21-30)	C_{256}	
4 (31-40)	C_{266}	
5 (41-50)	C_{333}	
6 (51-60)	C_{334}	
7 (61-70)	C_{335}	
8 (71-80)	C_{336}	

Card 11 (8E10.0) Third-Order Elastic Constants. Present only if TOSW ≠ 0 on Card 1.

Field	Variable Name	Description
1 (1-10)	C_{344}	Third-Order Elastic Constants
2 (11-20)	C_{345}	
3 (21-30)	C_{346}	
4 (31-40)	C_{355}	
5 (41-50)	C_{356}	
6 (51-60)	C_{366}	
7 (61-70)	C_{444}	
8 (71-80)	C_{445}	

Card 12 (8E10.0) Third-Order Elastic Constants. Present only if TOSW ≠ 0 on Card 1.

Field	Variable Name	Description
1 (1-10)	C_{446}	Third-Order Elastic Constants
2 (11-20)	C_{455}	
3 (21-30)	C_{456}	
4 (31-40)	C_{466}	
5 (41-50)	C_{555}	

Card 12 (8E10.0) Cont'd

Field	Variable Name	Description
6 (51-60)	C_{556}	Third-Order Elastic Constants
7 (61-70)	C_{566}	
8 (71-80)	C_{666}	

The elastic constants are symmetric with respect to any permutation of the indices. Only the independent (for a triclinic crystal) constants are read in. The constants are stored in a doubly subscripted array in the same order as read in. The first index picks the constant, and the second picks the material to which it applies. It may be noticed that for any second-order constant required in Equation (15), if its indices are permuted so that they are in increasing order, C_{ij}, where $i \leq j$, then the index of that constant in the storage array is

$$\text{Index} = L(i) + j \ ,$$

where L(1) = 0, L(2) = 5, L(3) = 9, L(4) = 12, L(5) = 15, L(6) = 15. For the third-order constants, the index of C_{ijk}, where $i \leq j \leq k$, is

$$\text{Index} = L1(i) + L(j) + k \ ,$$

where L(j) is as above, and L1(1) = 0, L1(2) = 15, L1(3) = 25, L1(4) = 31, L1(5) = 34, L1(6) = 35. This storage arrangement takes advantage of the symmetry of the constants and allows all constants to be referred to while storing only the independent constants.

Appendix B

Elastic Constants for α-Quartz

The elastic constants for α-quartz are as follows:[9,10]

(units are Mbars)

Second-Order

$C_{11} = .868$

$C_{12} = .0704$

$C_{13} = .1191$

$C_{14} = -.1804$

$C_{15} = 0$

$C_{16} = 0$

$C_{22} = .868$

$C_{23} = .1191$

$C_{24} = .1804$

$C_{25} = 0$

$C_{26} = 0$

$C_{33} = 1.0575$

$C_{34} = 0$

$C_{35} = 0$

$C_{36} = 0$

$C_{44} = .582$

$C_{45} = 0$

$C_{46} = 0$

$C_{55} = .582$

$C_{56} = -.1804$

$C_{66} = .3988$

Third-Order

$C_{111} = -2.1$

$C_{112} = -3.45$

$C_{113} = .12$

$C_{114} = -1.63$

$C_{115} = 0$

$C_{116} = 0$

$C_{122} = -2.23$

$C_{123} = -2.94$

$C_{124} = -.15$

$C_{125} = 0$

$C_{126} = 0$

$C_{133} = -3.12$

$C_{134} = .02$

$C_{135} = 0$

$C_{136} = 0$

$C_{144} = -1.34$

$C_{145} = 0$

$C_{146} = 0$

$C_{155} = -2.00$

$C_{156} = 1.04$

$C_{166} = -.5775$

$C_{222} = -3.32$

$C_{223} = .12$

$C_{224} = 1.93$

$C_{225} = 0$

$C_{226} = 0$

$C_{233} = -3.12$

$C_{234} = -.02$

$C_{235} = 0$

$C_{236} = 0$

$C_{244} = -2.00$

$C_{245} = 0$

$C_{246} = 0$

$C_{255} = -1.34$

$C_{256} = -.74$

$C_{266} = .6425$

$C_{333} = -8.15$

$C_{334} = 0$

$C_{335} = 0$

$C_{336} = 0$

$C_{344} = -1.1$

$C_{345} = 0$

$C_{346} = 0$

$C_{355} = -1.1$

$C_{356} = .02$

$C_{366} = 1.53$

$C_{444} = -2.76$

$C_{445} = 0$

$C_{446} = 0$

$C_{455} = 2.76$

$C_{456} = -.33$

$C_{466} = -.15$

$C_{555} = 0$

$C_{556} = 0$

$C_{566} = 0$

$C_{666} = 0$

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